**Supporting Information:**

**Formation of Lactic Acid (CH3CH(OH)COOH), a Metabolic Keystone for the Molecular Origins of Life, in** **Interstellar Ice Analogues**

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**Methods**

**Experimental**.The experiments were conducted in an ultrahigh vacuum chamber evacuated by magnetically suspended turbomolecular pumps (Osaka, TG1300MUCWB and TG420MCAB) and an oil-free scroll pump (XDS35i, BOC Edwards) at pressures of a few 10−11 Torr.[1](#_ENREF_1),[2](#_ENREF_2) A closed-cycle helium cryostat (Sumitomo Heavy Industries, RDK415E) was used to cool a polished silver substrate to temperatures as low as 5 K. The cryostat allows for vertical translation and horizontal rotation via an adjustable bellows (McAllister, BLT86) and a rotatable flange (Thermionics Vacuum Products, RNN-600/FA/MCO), respectively.[1](#_ENREF_1) The carbon dioxide samples used in the experiment included carbon dioxide (CO2,Airgas, 99.999%), carbon dioxide-13C (13CO2, Sigma-Aldrich, 99 atom % 13C), carbon dioxide-18O2 (C18O2, Sigma-Aldrich, 95 atom % 18O), and carbon dioxide-13C-18O2 (13C18O2, Sigma-Aldrich, 99 atom % 13C, 95 atom % 18O). Isotopically labeled ethanol sample—ethanol-d6 (CD3CD2OD; Cambridge Isotope Laboratories, 99 atom % D), ethanol-d3 (CD3CH2OD; Sigma Aldrich, 99 atom % D), ethanol-d2 (CH3CD2OD; CDN isotopes, 98.9 atom % D), or ethanol-13C2 (13CH313CH2OH; Sigma Aldrich, 99 atom % 13C)—was filled into a borosilicate vial interfaced with an ultrahigh vacuum chamber and subjected to several freeze-thaw cycles using liquid nitrogen to remove residual atmospheric gases. After the substrate was cooled to 4.9 ± 0.2 K, carbon dioxide gas and ethanol vapor were deposited separately onto the silver substrate via glass capillary arrays at partial pressures of 2 × 10−8 Torr for both carbon dioxide and ethanol. Although the temperature of 5 K is slightly below the typical 10–20 K range observed in cold molecular clouds, this lower temperature effectively immobilizes reactive species within the ice matrix, providing valuable mechanistic insights into the chemical processes occurring in such cold ices.[3](#_ENREF_3) Laser interferometry was used to monitor the ice thickness during deposition; interference fringes between reflections of the helium-neon laser (CVI Melles-Griot, 25-LHP-230, 632.8 nm) from the silver substrate and the ice surface were recorded using a photodiode.[4](#_ENREF_4) The thickness of the deposited CO2−CD3CD2OD ice was determined to be 950 ± 50 nm (Table S12), based on an average index (n) of 1.24 ± 0.04, derived from the indices of carbon dioxide ice (n = 1.21)[5](#_ENREF_5) at 10 K and that of ethanol ice (n = 1.26).[6](#_ENREF_6) Infrared spectra of the ice mixtures were collected using a Fourier transform infrared (FTIR) spectrometer (Thermo Electron, Nicolet 6700) over the range of 6000−500 cm−1 with a resolution of 4 cm−1 (Figures S1−S4, Tables S1−S4). FTIR spectra of pure ethanol-d3 (CD3CH2OH) ice and ethanol-d2 (CH3CD2OH) ice were recordedat 5 K with a thickness of 380 ± 50 nm (Figures S10–S11, Tables S8−S9). Utilizing the absorption bands of pure ethanol ices with known thickness, the thicknesses and column densities of ethanol-d6, ethanol-d3,ethanol-d2,and ethanol-13C2 in the ice mixtures were determined using the integrated area of multiple absorption bands.[7](#_ENREF_7) The ratio of carbon dioxide to ethanol in the CO2−CD3CD2OD ice was estimated to be 1.6 ± 0.3:1 (Table S12). Densities of 0.98 g cm−3 and 0.584 g cm−3 were used for CO2 and CH3CH2OH ices, respectively.[6](#_ENREF_6),[8](#_ENREF_8) Variations in density were used based on the masses of isotopically labeled carbon dioxide and ethanol molecules.

After the deposition, the ice mixtures were irradiated with energetic electrons (SPECS, EQ PU-22, 5 keV), simulating the secondary electrons produced by galactic cosmic rays (GCRs) as they pass through the interstellar ices.[7](#_ENREF_7) The CO2−CD3CD2OD ice was processed at an incidence angle of 70° with a current of 22 nA for 5 minutes, corresponding to doses of 0.21 ± 0.04 eV per CO2 molecule and 0.34 ± 0.06 eV per CD3CD2OD molecule, as calculated via Monte Carlo simulations using the CASINO software suite.[9](#_ENREF_9) These doses simulate secondary electrons generated in the track of GCRs in cold molecular clouds over timescales up to 7 × 105 years.[10](#_ENREF_10) The average penetration depth of electrons in CO2−CD3CD2OD ice was determined to be 370 ± 40 nm. Approximately 99% of the electron energy was deposited within the top 570 ± 50 nm of the ice, well below the total ice thickness of 950 ± 50 nm, thereby preventing interactions between the substrate and electrons. Infrared spectra of the ices were recorded *in situ* before, during, and after irradiation using the FTIR spectrometer. Following irradiation, the ices were heated from 5 to 320 K at a rate of 0.5 K min−1 during the temperature-programmed desorption (TPD) phase. During TPD, molecules released into the gas phase were photoionized by pulsed (30 Hz) vacuum ultraviolet (VUV) light, generated via resonant four-wave mixing in a noble gas jet. VUV photons at 11.10 eV were produced through sum frequency generation (2ω1 + ω2), whereas 10.54 eV and 9.34 eV photons were generated via difference frequency generation (2ω1 − ω2). The fundamental laser beam (ω1 or ω2) was produced by a tunable dye laser (Sirah Lasertechnik, Cobra-Stretch) pumped by an Nd:YAG laser (Spectra-Physics Quanta Ray PRO 270-30 or 250-30). Detailed VUV generation parameters are listed in Table S13. The VUV light was spatially separated from the fundamental laser beams using a biconvex lithium fluoride lens (Korth Kristalle, R = 131 mm) in an off-axis geometry and was directed 2.0 ± 0.5 mm above the ice surface to ionize the subliming molecules in the gas phase. The VUV photon flux was monitored during TPD with a Faraday cup and used to correct for fluctuations in the TPD profiles. The resulting ions were mass-analyzed using a reflectron time-of-flight mass spectrometer (ReToF-MS, Jordan TOF Products) and detected with a dual microchannel plate (MCP) detector. The ion signals were amplified, discriminated, and recorded with a multichannel scaler (FAST ComTec, MCS6A). Each mass spectrum featured an ion arrival time resolution of 3.2 ns and an accumulation time of 2 minutes with 3600 sweeps. Note that C2H2O4 isomers (90 amu) may be formed via the recombination of two hydroxycarbonyl (HOĊO) radicals, whereas C4H10O2 isomers (90 amu) can result from the recombination of radicals generated from ethanol (CH3CH2OH). To distinguish these species from C3H6O3 isomers (90 amu), fully deuterated CO2−CD3CD2OD ices were employed, facilitating clear mass spectrometric differentiation of the isomeric products. A gas phase mass spectrum of L-(+)-lactic acid (C3H6O3, Sigma-Aldrich, ≥ 98%) was measured at a photon energy of 11.10 eV (Figure S8).

**Computational**.The energies and geometries of all the neutral and cationic states of conformers were calculated using the CBS-QB3 composite scheme, which provides accuracy of 4−8 kJ for relative energies, 0.01−0.02 Å for bond lengths, and 1−2° for bond angles. All calculations were performed in the GAUSSIAN 09 software package.[11](#_ENREF_11) Three reaction products—lactic acid (**1**), monoethyl carbonate (**15**), and 3-hydroxypropanoic acid (**16**)—are evaluated for the computational study, reflecting their formation under low-dose irradiation conditions. Each backbone isomer has a number of conformational isomers arising from rotations around single bonds that differ in energies and ionization potentials. To obtain accurate ranges on ionization potentials, it was important to consider all possible conformational isomers, and we generated geometries of all possible conformers for each backbone isomer. Firstly, CBS-QB3 composite scheme calculations were carried out for neutral conformers, which includes geometry optimization and energy evaluation. Then the same procedure was applied for their cations, with their initial geometries taken from the corresponding neutral conformers. Among all considered isomers, monoethyl carbonate (**15**) has the lowest energy with 4 conformers and has the highest ionization potential (Table S6). In comparison with **15**, lactic acid (**1**) and 3-hydroxypropanoic acid (**16**) have slightly higher energies (by 12–56 kJ mol−1), with 10 and 20 conformers identified, respectively (Tables S5 and S7). The Cartesian coordinates, harmonic vibrational frequencies, and infrared intensities of all computed structures are provided in Table S14.

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**Figure S1.** Infrared spectra of (**a**) CO2−CD3CD2OD ice before and after irradiation at 5 K with (**b**) a magnified view and deconvolution (Gaussian) of the region 1900–1500 cm−1 of the difference spectrum. The assignments of the absorptions of CO2, CD3CD2OD, and new absorptions after irradiation are labeled in magenta, black, and red, respectively. Detailed assignments are compiled in Table S1.

A graph of different types of data

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**Figure S2.** Infrared spectra of (**a**) 13CO2−13CH313CH2OH ice before and after irradiation at 5 K with (**b**) a magnified view and deconvolution (Gaussian) of the region 1900–1500 cm−1 of the difference spectrum. The assignments of the absorptions of 13CO2, 13CH313CH2OH, and new absorptions after irradiation are labeled in magenta, black, and red, respectively. Detailed assignments are compiled in Table S2.

A graph of different types of data

Description automatically generated with medium confidence**Figure S3.** Infrared spectra of (**a**) C18O2−CH3CD2OH ice before and after irradiation at 5 K with (**b**) a magnified view and deconvolution (Gaussian) of the region 1900–1500 cm−1 of the difference spectrum. The assignments of the absorptions of C18O2, CH3CD2OH, and new absorptions after irradiation are labeled in magenta, black, and red, respectively. Detailed assignments are compiled in Table S3.

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Description automatically generated with medium confidence

**Figure S4.** Infrared spectra of (**a**) 13C18O2−CD3CH2OH ice before and after irradiation at 5 K with (**b**) a magnified view and deconvolution (Gaussian) of the region 1900–1500 cm−1 of the difference spectrum. The assignments of the absorptions of 13C18O2, CD3CH2OH, and new absorptions after irradiation are labeled in magenta, black, and red, respectively. Detailed assignments are compiled in Table S4.

A graph of a graph showing a graph of a molecule

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**Figure S5.** Difference inTPD profiles of *m/z* = 96 measured at photon energies of 11.10 eV and 10.54 eV from irradiated CO2–CD3CD2OD ice.

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**Figure. S6.** Proposed formation pathways of isomers **1** (*m/z* = 95, 96, and 97), **15** (*m/z* = 96 and 97), and **16** (*m/z* = 96 and 97) via radical–radical reactions in carbon dioxide-18O2–ethanol-d2 (C18O2–CH3CD2OH) ice after electron irradiation.

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AI-generated content may be incorrect.

**Figure. S7.** Proposed formation pathways of isomers **1** (*m/z* = 98 and 99), **15** (*m/z* = 98 and 99), and **16** (*m/z* = 97 and 98) via radical–radical reactions in carbon dioxide-13C-18O2–ethanol-d3 (13C18O2–CD3CH2OH) ice after electron irradiation.

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Description automatically generated with medium confidence

**Figure S8**. Gas phase mass spectra of lactic acid (C3H6O3,*m/z* = 90) recorded at a VUV photon energy of 11.10 eV, showing a significant fragment signal of *m/z* = 45. Mass spectra were collected for background gases with 10800 laser pulses (a) and lactic acid at a pressure of 3 ×10−9 Torr with 30030 laser pulses (b).

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**Figure** **S9.** TPD profiles of *m/z* = 46, 50, and 96 in irradiated CO2–CD3CD2OD ice measured at 11.10 eV.

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**Figure S10.** Infrared spectra of CH3CD2OH ice with a thickness of 380 ± 50 nm. The assignments of the absorptions are deconvoluted with Gaussian peaks and labeled in blue and green. Detailed assignments are compiled in Table S10.

A graph of a scientific experiment

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**Figure S11.** Infrared spectra of CD3CH2OH ice with a thickness of 380 ± 50 nm. The assignments of the absorptions are deconvoluted with Gaussian peaks and labeled in blue and green. Detailed assignments are compiled in Table S11.

**Table S1.** Observed absorption peaks of CO2−CD3CD2OD ice before and after irradiation at 5 K. Vibration mode: stretching (*ν*), bending (*δ*), wagging (*ω*), and rocking (*ρ*). Indication: asymmetric (*a*) and symmetric (*s*).

|  |  |
| --- | --- |
| Pristine ice, absorptions before irradiation (cm−1) |  |
| **CO2** | Assignment[8](#_ENREF_8" \o "Bouilloud, 2015 #1437) |
| 3700 | *ν*1 + *ν*3 |
| 3593 | 2*ν*2 + *ν*3 |
| 2349 | C-O asymmetric stretching (*ν*3) |
| 2277 | C-O asymmetric stretching (*ν*3 (13CO2)) |
| **CD3CD2OD** | Assignment[12](#_ENREF_12" \o "Mikawa, 1971 #3111) |
| 3626 | *ν*(OD) + *νa*(CD3) |
| 3435, 3353, 3255 | *ν*(OH) |
| 2672 | *ν*(OD)D |
| 2547, 2505, 2438 | *ν*(OD) |
| 2233 | *νa*(CD3) |
| 2175 | *νs*(CD3) |
| 2106 | *νs*(CD2) |
| 2075 | 2*νa*(CD3) |
| 1224 | *γ*(OD) + *ρ*(CD3) |
| 1184 | *ν*(CO) |
| 1124 | *δs*(CD2) |
| 1092 | *ω*(CD2) |
| 1071, 1046 | *δ'a*(CD3) |
| 1020, 967 | *δa*(CD3) |
| 906 | *ν*(CC) |
| 739 | *ρ*(CD3) |
| New absorptions after irradiation (cm−1) | Assignment[13-15](#_ENREF_13) |
| 1764 | *ν*2(DOĊO) |
| 1684 | *ν*2(D2CO) |
| 1642 | C=O stretch |

**Table S2.** Observed absorption peaks of 13CO2−13CH313CH2OH ice before and after irradiation at 5 K. Vibration mode: stretching (*ν*), bending (*δ*), torsion (*τ*), wagging (*ω*), and rocking (*ρ*). Indication: asymmetric (*a*) and symmetric (*s*).

|  |  |
| --- | --- |
| Pristine ice, absorptions before irradiation (cm−1) |  |
| **13CO2** | Assignment[2](#_ENREF_2" \o "Wang, 2024 #3316) |
| 3620 | *ν*1 + *ν*3 |
| 3507 | 2*ν*2 + *ν*3 |
| 2343 | C-O asymmetric stretching (*ν*3 (CO2)) |
| 2282 | C-O asymmetric stretching (*ν*3) |
| **13CH313CH2OH** | Assignment[7](#_ENREF_7" \o "Wang, 2024 #3405) |
| 3414, 3316, 3215 | *ν*(OH) |
| 2969 | *νa*(13CH3) |
| 2932 | *νs*(13CH3) |
| 2887, 2833 | *νs*(13CH2) |
| 2733 | *ω*(13CH2) + *δ*(OH) |
| 2676 | *δs*(13CH3) + *δ*(OH) |
| 2382 | *δ*(OH) + *ρ*(13CH3) |
| 1885 | *ν*(13CO) + *ν*(13CC) |
| 1480 | *δs*(13CH2) |
| 1451 | *δa*(13CH3) |
| 1418 | *ω*(13CH2) |
| 1369 | *δs*(13CH3) |
| 1324 | *δ*(OH) |
| 1261 | *τ*(13CH2) |
| 1069 | *ρ*(13CH3) |
| 1024 | *ν*(13CO) |
| 869 | *ν*(13C13C) |
| New absorptions after irradiation (cm−1) | Assignment[2](#_ENREF_2),[15](#_ENREF_15),[16](#_ENREF_16) |
| 2092 | *ν*(13CO) |
| 1702 | *ν*2(H213CO) |
| 1673 | *ν*4(13CH313CHO) |
| 1605 | 13C=O stretch |

**Table S3.** Observed absorption peaks of C18O2−CH3CD2OH ice before and after irradiation at 5 K. Vibration mode: stretching (*ν*), bending (*δ*), torsion (*τ*), and wagging (*ω*). Indication: asymmetric (*a*) and symmetric (*s*).

|  |  |
| --- | --- |
| Pristine ice, absorptions before irradiation (cm−1) |  |
| **C18O2** | Assignment[2](#_ENREF_2) |
| 3620 | *ν*1 + *ν*3 |
| 3510 | 2*ν*2 + *ν*3 |
| 2315 | C-18O asymmetric stretching (*ν*3) |
| 2242 | C-18O asymmetric stretching (*ν*3 (13C18O2)) |
| **CH3CD2OH** | Assignment[12](#_ENREF_12),[17](#_ENREF_17) |
| 3417, 3323, 3191 | *ν*(OH) |
| 2974 | *νa*(CH3) |
| 2937 | *νs*(CH3) |
| 2903, 2870 | *νs*(CD2) |
| 2793 | *ω*(CD2) + *δ*(OH) |
| 2242 | 2*δs*(CD2) |
| 2198 | 2*ω*(CD2) |
| 2126 | *δ*(OD) + *δs*(CD2) |
| 2098 | *ν*(CO) + *δs*(CD2) |
| 1465 | *δ'a*(CH3) |
| 1446 | *δa*(CH3) |
| 1374 | *δs*(CH3) |
| 1300 | *δ*(OH) |
| 1160 | *δs*(CD2) |
| 1129 | *ω*(CD2) |
| 1027 | *ν*(CO) |
| 962 | *δ*(OD) |
| 912, 850 | *ν*(CC) |
| New absorptions after irradiation (cm−1) | Assignment[13](#_ENREF_13),[18](#_ENREF_18) |
| 1715 | *ν*4(CH3CHO) |
| 1680 | *ν*2(D2CO) |
| 1622 | C=18O stretch |

**Table S4.** Observed absorption peaks of 13C18O2−CD3CH2OH ice before and after irradiation at 5 K. Vibration mode: stretching (*ν*), bending (*δ*), torsion (*τ*), wagging (*ω*), and rocking (*ρ*). Indication: asymmetric (*a*) and symmetric (*s*).

|  |  |
| --- | --- |
| Pristine ice, absorptions before irradiation (cm−1) |  |
| **13C18O2** | Assignment |
| 3621 | *ν*1 + *ν*3 |
| 3530 | 2*ν*2 + *ν*3 |
| 2310 | C-18O asymmetric stretching (*ν*3 (C18O2)) |
| 2249 | 13C-18O asymmetric stretching (*ν*3) |
| **CD3CH2OH** | Assignment[12](#_ENREF_12),[17](#_ENREF_17) |
| **3431** | *νs*(CD3) + *τ*(CH2) |
| 3426, 3334, 3211 | *ν*(OH) |
| 2975 | *νa*(CH2) |
| 2941 | 2*δs*(CH2) |
| 2895 | *νs*(CH2) |
| 2731 | *ω*(CH2) + *δ*(OH) |
| 2196 | *νs*(CD3) |
| 2126 | 2*δ'a*(CD3) |
| 2085 | *δ*(OH) + *ρ*(CD3) |
| 1487 | *δs*(CH2) |
| 1433 | *ω*(CH2) |
| 1390 | *γ*(OH) *+ ρ*(CD3) |
| 1320 | *δ*(OH) |
| 1246 | *τ*(CH2) |
| 1135 | *ν*(CO) |
| 1065 | *δ'a*(CD3) |
| 1031 | *δa*(CD3) |
| 939 | *ρ'*(CD3) |
| 755 | *ρ*(CD3) |
| New absorptions after irradiation (cm−1) | Assignment[18](#_ENREF_18),[19](#_ENREF_19) |
| 2040 | *ν*(13C18O) |
| 1706 | *ν*4(CD3CHO) |
| 1578 | 13C=18O stretch |

**Table S5.** Error analysis of adiabatic ionization energies (IEs) and relative energies (ΔE) of lactic acid (**1**) conformers computed at the composite CBS-QB3 level including the zero-point vibrational energy (ZPVE) corrections. The IE ranges are corrected for the thermal and Stark effect by −0.03 eV and the combined error limits of −0.05/+0.05 eV.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Conformer | Structure | ΔE  (kJ mol-1) | Computed IE (eV) | Corrected IE ranges (eV) |
| **1a** |  | 14 | 9.95 | 9.87–9.97 |
| **1b** |  | 12 | 9.97 | 9.89–9.99 |
| **1c** |  | 13 | 9.97 | 9.89–9.99 |
| **1d** |  | 20 | 9.90 | 9.82–9.92 |
| **1e** |  | 14 | 9.97 | 9.89–9.99 |
| **1f** |  | 10 | 10.04 | 9.96–10.06 |
| **1g** |  | 10 | 10.04 | 9.96–10.06 |
| **1h** |  | 0 | 10.16 | 10.08–10.18 |
| **1i** |  | 21 | 9.95 | 9.87–9.97 |
| **1j** |  | 20 | 9.96 | 9.88–9.98 |

**Table S6.** Error analysis of adiabatic ionization energies (IEs) and relative energies (ΔE) of monoethyl carbonate (**15**) conformers computed at the composite CBS-QB3 level including the zero-point vibrational energy (ZPVE) corrections. The IE ranges are corrected for the thermal and Stark effect by −0.03 eV and the combined error limits of −0.05/+0.05 eV.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Conformer | Structure | ΔE  (kJ mol-1) | Computed IE (eV) | Corrected IE ranges (eV) |
| **15a** | A molecule model of a chemical structure  AI-generated content may be incorrect. | 14 | 10.61 | 10.53–10.63 |
| **15b** | A red and grey molecule  AI-generated content may be incorrect. | 0 | 10.76 | 10.68–10.78 |
| **15c** | A molecule model of a chemical compound  AI-generated content may be incorrect. | 5 | 10.70 | 10.62–10.72 |
| **15d** | A molecule model of a chemical compound  AI-generated content may be incorrect. | 42 | 10.53 | 10.45–10.55 |

**Table S7.** Error analysis of adiabatic ionization energies (IEs) and relative energies (ΔE) of 3-hydroxypropanoic acid (**16**) conformers computed at the composite CBS-QB3 level including the zero-point vibrational energy (ZPVE) corrections. The IE ranges are corrected for the thermal and Stark effect by −0.03 eV and the combined error limits of −0.05/+0.05 eV.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Conformer | Structure | ΔE  (kJ mol-1) | Computed IE (eV) | Corrected IE ranges (eV) |
| **16a** |  | 12 | 9.27 | 9.19–9.29 |
| **16b** |  | 32 | 9.19 | 9.11–9.21 |
| **16c** |  | 28 | 9.23 | 9.15–9.25 |
| **16d** |  | 32 | 9.19 | 9.11–9.21 |
| **16e** |  | 28 | 9.23 | 9.15–9.25 |
| **16f** |  | 0 | 9.89 | 9.81–9.91 |
| **16g** |  | 8 | 9.99 | 9.91–10.01 |
| **16h** |  | 16 | 10.05 | 9.97–10.07 |
| **16i** |  | 19 | 10.08 | 10.00–10.10 |
| **16j** |  | 20 | 10.13 | 10.05–10.15 |
| **16k** |  | 28 | 10.04 | 9.96–10.06 |
| **16l** |  | 16 | 10.22 | 10.14–10.24 |
| **16m** |  | 36 | 10.06 | 9.98–10.08 |
| **16n** |  | 13 | 10.31 | 10.23–10.33 |
| **16o** |  | 12 | 10.32 | 10.24–10.34 |
| **16p** |  | 9 | 10.48 | 10.40–10.50 |
| **16q** |  | 11 | 10.46 | 10.38–10.48 |
| **16r** |  | 14 | 10.44 | 10.36–10.46 |
| **16s** |  | 15 | 10.43 | 10.35–10.45 |
| **16t** |  | 37 | 10.43 | 10.35–10.45 |

**Table S8.** Error analysis of IEs and relative energies (ΔE) of prop-1-ene-1,1,2-triol (CH3C(OH)C(OH)2, **19**) conformers computed at the composite CBS-QB3 level including the zero-point vibrational energy (ZPVE) corrections. The IE ranges are corrected for the thermal and Stark effect by −0.03 eV and the combined error limits of −0.05/+0.05 eV.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Conformer | Structure | ΔE  (kJ mol-1) | Computed IE (eV) | Corrected IE ranges (eV) |
| **19a** |  | 0 | 7.46 | 7.38–7.48 |
| **19b** |  | 8 | 7.54 | 7.46–7.56 |
| **19c** |  | 12 | 7.57 | 7.49–7.59 |
| **19d** |  | 3 | 7.69 | 7.61–7.71 |
| **19e** |  | 20 | 7.53 | 7.45–7.55 |

**Table S9.** Error analysis of IEs and relative energies (ΔE) of prop-1-ene-1,1,3-triol (HOCH2CHC(OH)2, **20**) conformers computed at the composite CBS-QB3 level including the zero-point vibrational energy (ZPVE) corrections. The IE ranges are corrected for the thermal and Stark effect by −0.03 eV and the combined error limits of −0.05/+0.05 eV.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Conformer | Structure | ΔE  (kJ mol-1) | Computed IE (eV) | Corrected IE ranges (eV) |
| **20a** |  | 4 | 7.93 | 7.85–7.95 |
| **20b** |  | 0 | 7.98 | 7.90–8.00 |
| **20c** |  | 4 | 7.93 | 7.85–7.95 |
| **20d** |  | 8 | 8.08 | 8.00–8.10 |
| **20e** |  | 12 | 8.03 | 7.95–8.05 |
| **20f** |  | 17 | 8.27 | 8.19–8.29 |
| **20g** |  | 15 | 8.39 | 8.31–8.41 |
| **20h** |  | 18 | 8.40 | 8.32–8.42 |
| **20i** |  | 24 | 8.36 | 8.28–8.38 |
| **20j** |  | 24 | 8.35 | 8.27–8.37 |
| **20k** |  | 27 | 8.32 | 8.24–8.34 |
| **20l** |  | 28 | 8.31 | 8.23–8.33 |
| **20m** |  | 12 | 8.50 | 8.42–8.52 |
| **20n** |  | 21 | 8.46 | 8.38–8.48 |
| **20o** |  | 28 | 8.42 | 8.34–8.44 |

**Table S10.** Observed absorption peaks of ethanol-d2 (CH3CD2OH) ice at 5 K. Vibration mode: stretching (*ν*), bending (*δ*), and wagging (*ω*). Indication: asymmetric (*a*) and symmetric (*s*).

|  |  |
| --- | --- |
| Pristine ice, absorptions (cm−1) |  |
| **CH3CD2OH** | Assignment[12](#_ENREF_12),[17](#_ENREF_17) |
| 3421, 3314, 3179 | *ν*(OH) |
| 2970 | *νa*(CH3) |
| 2935 | *νs*(CH3) |
| 2905, 2869 | *νs*(CD2) |
| 2791 | *ω*(CD2) + *δ*(OH) |
| 2508 | *ν*(OD) |
| 2249 | 2*δs*(CD2) |
| 2189 | 2*ω*(CD2) |
| 2121 | *δ*(OD) + *δs*(CD2) |
| 2095 | *ν*(CO) + *δs*(CD2) |
| 1465 | *δ'a*(CH3) |
| 1446 | *δa*(CH3) |
| 1371 | *δs*(CH3) |
| 1335 | *δ*(OH) |
| 1163 | *δs*(CD2) |
| 1126 | *ω*(CD2) |
| 1025 | *ν*(CO) |
| 963 | *δ*(OD) |
| 910, 853 | *ν*(CC) |

**Table S11.** Observed absorption peaks of ethanol-d3 (CD3CH2OH) ice at 5 K. Vibration mode: stretching (*ν*), bending (*δ*), torsion (*τ*), wagging (*ω*), and rocking (*ρ*). Indication: asymmetric (*a*) and symmetric (*s*).

|  |  |
| --- | --- |
| Pristine ice, absorptions (cm−1) |  |
| **CD3CH2OH** | Assignment[12](#_ENREF_12),[17](#_ENREF_17) |
| 3421, 3314, 3179 | *ν*(OH) |
| 2969 | *νa*(CH2) |
| 2887 | *νs*(CH2) |
| 2741 | *ω*(CH2) + *δ*(OH) |
| 2230 | *νa*(CD3) |
| 2199 | *νs*(CD3) |
| 2121 | 2*δ'a*(CD3) |
| 2082 | *δ*(OH) + *ρ*(CD3) |
| 1486 | *δs*(CH2) |
| 1436 | *ω*(CH2) |
| 1372 | γ(OH) *+ ρ*(CD3) |
| 1320 | *δ*(OH) |
| 1251 | *τ*(CH2) |
| 1135 | *ν*(CO) |
| 1066 | *δ'a*(CD3) |
| 939 | *ρ'*(CD3) |
| 757 | *ρ*(CD3) |

**Table S12.** Experimental conditions of carbon dioxide−ethanol ices including composition, ice thickness, irradiation current and time, and photon energy.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Ice | Composition of carbon dioxide to ethanol | Thickness (nm) | Current  (nA) | Irradiation  time (s) | Dose (eV/ carbon dioxide) | Dose (eV/ ethanol) | Photon energy (eV) |
| CO2−CD3CD2OD | 1.6 ± 0.3 : 1 | 950 ± 50 | − | − | − | − | 11.10 |
| CO2−CD3CD2OD | 1.6 ± 0.2 : 1 | 920 ± 50 | 22 ± 1 | 300 ± 10 | 0.21 ± 0.04 | 0.34 ± 0.06 | 11.10 |
| CO2−CD3CD2OD | 1.2 ± 0.4 : 1 | 900 ± 50 | 23 ± 1 | 300 ± 10 | 0.22 ± 0.04 | 0.35 ± 0.06 | 10.54 |
| CO2−CD3CD2OD | 1.6 ± 0.3 : 1 | 950 ± 50 | 22 ± 1 | 300 ± 10 | 0.21 ± 0.04 | 0.34 ± 0.06 | 9.34 |
| 13CO2−13CH313CH2OH | 1.4 ± 0.6 : 1 | 920 ± 50 | 22 ± 1 | 300 ± 10 | 0.21 ± 0.04 | 0.31 ± 0.05 | 11.10 |
| C18O2−CH3CD2OH | 1.2 ± 0.3 : 1 | 920 ± 50 | 21 ± 1 | 300 ± 10 | 0.22 ± 0.04 | 0.31 ± 0.05 | 11.10 |
| 13C18O2−CD3CH2OH | 1.3 ± 0.2 : 1 | 920 ± 50 | 24 ± 1 | 300 ± 10 | 0.25 ± 0.04 | 0.32 ± 0.05 | 11.10 |

**Table S13.** Generation parameters of vacuum ultraviolet light with a photon energy uncertainty of less than 0.001 eV.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| VUV photon energy (eV) | Nonlinear medium in four-wave mixing | Laser wavelength for ω1 (nm) | Dye for ω1 | Laser wavelength for ω2 (nm) | Dye for ω2 |
| 11.10  (2ω1 + ω2) | Xenon | 249.628 | Coumarin 503 | 1064 | − |
| 10.54  (2ω1 − ω2) | Krypton | 202.316 | Rhodamine 610 and 640 | 722.321 | LDS 722 |
| 9.34  (2ω1 − ω2) | Krypton | 212.556 | Stilbene 420 | 532 | − |

**Table S14.** Cartesian coordinates (Å), harmonic frequencies (cm−1), and infrared intensities (km mol−1) of isomers **1**, **15**, and **16** calculated at the composite CBS-QB3 level of theory.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **1a**  O 1.352704 -1.287671 -0.053042  C 0.839223 -0.203008 -0.054794  C -0.646416 0.023709 -0.399577  C -1.545208 -1.022119 0.242751  O 1.515645 0.927208 0.210549  O -1.035049 1.371575 -0.083710  H -0.716528 -0.048554 -1.489466  H -1.522008 -0.935492 1.334554  H -2.574686 -0.902676 -0.099909  H -1.192389 -2.020496 -0.015105  H 0.870371 1.654278 0.147896  H -1.416757 1.372556 0.801374  Freq Int   |  |  | | --- | --- | | 69.9431 232.4339 265.2626 344.0584 347.7646 416.5937 519.7772 566.8145 736.6324 761.7481 816.8751 906.7986 1054.9033 1074.4069 1130.9969 1198.0989 1287.9706 1335.8072 1391.9398 1398.9051 1409.3302 1493.0763 1496.7878 1858.2913 3027.1448 3051.8733 3100.1344 3136.0255 3646.1715 3811.7566 | 6.0568 0.588 17.4379 55.0699 55.7965 7.6255 1.8136 12.6245 11.5798 83.5524 16.5803 8.8506 55.2255 22.6889 40.8991 45.4032 2.6912 29.1977 328.4264 88.1789 35.6671 7.3148 10.4684 254.2846 12.1092 14.0676 23.7564 5.5768 146.2047 32.7884 | | **1a+**  O 1.208793 -1.400314 0.025094  C 0.972003 -0.250520 -0.016663  C -0.798167 0.138838 -0.399115  C -1.687488 -0.922573 0.160130  O 1.690232 0.808005 0.101149  O -0.929550 1.409334 0.028694  H -0.623494 0.131619 -1.480529  H -1.694653 -0.925228 1.253933  H -2.706294 -0.723617 -0.193717  H -1.385673 -1.907604 -0.194268  H 1.157373 1.625301 0.042790  H -1.421147 1.468861 0.866189  Freq Int   |  |  | | --- | --- | | 80.4994 196.5917 227.6315 240.007 332.9677 385.9162 450.7592 531.0747 592.4454 623.454 684.2799 912.888 994.041 1057.035 1154.4423 1198.3688 1226.7333 1264.3899 1330.5158 1404.5641 1434.0147 1463.5124 1475.2557 1914.1239 3023.6946 3060.6557 3091.773 3144.923 3633.8244 3705.6502 | 2.5532 7.4082 9.4784 1.8404 3.9385 15.1718 8.2332 22.7863 77.2125 85.5211 76.8671 29.8742 22.6767 60.0549 19.7098 73.0798 54.2224 396.3114 33.0178 11.4304 84.6565 10.5842 12.0677 133.0194 18.2214 18.3329 5.9238 2.1925 129.3304 209.1272 | |
| **1b**  O 1.504635 -1.123274 -0.243350  C 0.851542 -0.129713 -0.081736  C -0.646477 -0.078804 -0.416412  C -1.417677 -1.092335 0.424605  O 1.361749 1.008308 0.412530  O -1.086556 1.267954 -0.200031  H -0.733123 -0.333656 -1.479348  H -1.352874 -0.835756 1.484982  H -2.471613 -1.115503 0.131657  H -0.997319 -2.088009 0.278989  H 0.639142 1.658959 0.444842  H -2.047170 1.295178 -0.173054  Freq Int   |  |  | | --- | --- | | 48.6999 141.145 252.9766 264.4809 352.2804 411.0907 527.4241 599.5752 688.2346 740.456 813.0866 908.2761 1042.0318 1100.8906 1128.108 1163.4718 1267.3062 1349.5133 1388.122 1401.4751 1408.4049 1493.9863 1499.462 1861.1984 3022.4711 3030.2754 3096.2631 3127.7055 3672.5448 3850.3049 | 32.0876 103.5598 4.7691 8.4579 15.023 12.0168 2.753 13.7965 82.3272 6.7591 5.713 9.105 8.0383 8.9875 80.5541 94.4328 16.5554 59.1433 104.3612 160.429 142.0337 5.9603 11.3974 266.825 21.5874 18.0165 25.1755 7.761 150.2754 34.2519 | | **1b+**  O 1.208264 -1.400494 0.025202  C 0.971533 -0.250586 -0.016697  C -0.797701 0.138865 -0.398996  C -1.687713 -0.922189 0.160024  O 1.690444 0.807516 0.101073  O -0.929056 1.409532 0.028731  H -0.623464 0.131698 -1.480528  H -1.694766 -0.925106 1.253830  H -2.706403 -0.722559 -0.193707  H -1.386449 -1.907327 -0.194562  H 1.158073 1.625142 0.042879  H -1.420927 1.469173 0.866054  Freq Int   |  |  | | --- | --- | | 80.6307 196.8373 227.7788 240.1759 333.1686 386.1077 450.7965 531.156 592.3952 623.5354 684.3993 912.8525 994.1565 1056.9784 1154.4907 1198.4259 1226.6583 1264.5137 1330.3336 1404.5753 1433.9159 1463.492 1475.2627 1913.2292 3023.806 3060.1743 3091.8263 3144.8612 3633.8636 3705.6857 | 2.5526 7.4324 9.4796 1.8337 3.9273 15.1756 8.2203 22.7452 77.4681 85.7502 76.5293 29.8683 22.6406 60.086 20.0346 73.5177 53.649 395.65 33.0518 11.4373 84.5367 10.62 11.99 132.9816 18.2132 18.4389 5.8747 2.1969 129.2023 209.3495 | |
| **1c**  O -1.401138 1.231547 -0.154400  C -0.840239 0.174147 -0.069865  C 0.655048 0.012645 -0.387398  C 1.493582 1.065878 0.327730  O -1.466424 -0.957841 0.285230  O 1.025084 -1.324652 -0.019416  H 0.741648 0.139059 -1.474488  H 1.444086 0.914602 1.408192  H 2.539028 1.004803 0.014241  H 1.113440 2.061075 0.094711  H -0.797744 -1.664598 0.296068  H 1.849026 -1.563398 -0.452846  Freq Int   |  |  | | --- | --- | | 65.9481 167.9287 227.6287 269.5995 354.6307 421.3235 527.2558 577.2778 689.0315 741.8489 813.2069 909.5446 1040.8966 1114.7021 1124.6876 1165.107 1246.5326 1341.051 1398.0193 1403.273 1408.9481 1490.592 1498.6116 1860.5448 3008.6534 3038.5033 3105.3204 3130.2986 3668.868 3855.9606 | 8.0013 111.8085 0.7263 14.1287 12.6752 9.9187 4.7713 11.2069 92.4331 9.3684 4.3965 8.7067 6.7274 49.6263 24.6226 110.2421 16.6965 65.9424 160.833 133.7078 104.016 10.4879 6.5012 262.539 23.1724 17.0395 23.6895 8.5178 153.9194 42.8241 | | **1c+**  O -1.594410 0.952605 -0.508711  C -0.965988 0.061241 -0.065761  C 0.810014 0.148987 -0.452992  C 1.334712 1.075816 0.610897  O -1.270700 -0.949699 0.667655  O 1.224508 -1.131061 -0.321653  H 0.785263 0.530789 -1.473769  H 1.247011 0.652379 1.613415  H 2.403147 1.213415 0.399428  H 0.839920 2.045291 0.563899  H -0.502383 -1.535485 0.818004  H 1.279429 -1.597415 -1.172173  Freq Int   |  |  | | --- | --- | | 80.5097 189.7771 227.48 240.8399 276.7111 429.657 517.7526 533.365 567.5335 632.5561 693.7957 899.3361 995.3795 1045.5469 1133.7353 1191.8328 1231.4733 1266.77 1291.4612 1396.9004 1434.9093 1462.6349 1471.4518 1887.3117 3015.5625 3097.7922 3124.3585 3152.1956 3625.7093 3726.9211 | 3.2469 2.1852 2.2549 7.4733 15.464 4.0974 15.9439 90.3077 13.4022 91.2734 69.8941 15.5883 15.0088 37.6824 80.8436 61.546 6.6499 297.7147 167.371 13.4262 0.6498 23.4228 14.2511 119.7307 33.7331 4.4367 3.8513 1.059 114.7971 262.1643 | |
| **1d**  O 1.228585 -1.158883 -0.419502  C 0.806200 -0.122744 0.018623  C -0.666492 0.055328 0.402430  C -1.342523 1.159880 -0.421151  O 1.619257 0.939619 0.192342  O -1.342668 -1.164370 0.223828  H -0.692197 0.333950 1.468158  H -1.257288 0.939611 -1.487288  H -2.401260 1.193249 -0.160839  H -0.916344 2.150079 -0.230633  H 1.126089 1.684026 0.558446  H -0.683501 -1.786637 -0.120596  Freq Int   |  |  | | --- | --- | | 57.93 226.0397 260.8474 321.4419 374.4772 418.6081 478.8067 500.4001 632.5042 736.035 810.6313 927.3391 1046.744 1104.3909 1157.5031 1187.4501 1272.571 1313.0732 1361.046 1414.1214 1432.6902 1487.3868 1502.2578 1844.4282 2959.8171 3029.2149 3098.3439 3123.0093 3707.5611 3804.767 | 0.1886 0.2091 6.5649 23.822 96.9362 2.1269 102.9052 2.7608 9.5334 6.7715 4.1348 6.3779 22.0229 25.9986 99.087 32.3421 5.5196 447.4691 2.7553 6.455 14.6437 8.975 10.0192 241.4703 40.699 20.6176 27.8267 12.8762 92.9871 45.7701 | | **1d+** (same as **1c+**) |
| **1e**  O 1.572706 -1.038825 -0.326625  C 0.857209 -0.105892 -0.087399  C -0.648803 -0.112756 -0.407170  C -1.373299 -1.133226 0.462778  O 1.289438 1.021522 0.501571  O -1.214069 1.191209 -0.168881  H -0.746845 -0.387289 -1.461606  H -1.308859 -0.843260 1.514330  H -2.426339 -1.184284 0.181511  H -0.916219 -2.116037 0.341759  H 0.511431 1.603828 0.576617  H -1.308405 1.647030 -1.010389  Freq Int   |  |  | | --- | --- | | 44.0434 240.8132 256.7838 271.7737 339.0585 399.4174 521.9908 619.9666 731.1142 775.137 810.8387 909.6865 1047.9724 1064.6567 1108.6014 1217.3359 1262.0142 1310.8896 1383.4091 1403.8057 1409.9797 1489.4055 1498.6757 1861.5749 3043.2685 3052.9235 3114.374 3131.7008 3637.5817 3847.3584 | 9.0884 6.7757 3.8196 104.7923 3.3048 8.8675 3.9666 8.5305 30.1784 64.8699 7.5778 10.4696 78.1279 22.9348 23.6318 20.9846 56.5224 9.9683 109.1592 296.4411 9.244 12.1784 2.9124 264.9643 8.9435 16.3915 21.5537 9.9421 149.7653 54.5177 | | **1e+**  O 1.594105 -0.952181 -0.508998  C 0.965326 -0.061092 -0.065824  C -0.809266 -0.149127 -0.452995  C -1.334191 -1.075794 0.611054  O 1.270117 0.949480 0.668088  O -1.224243 1.130901 -0.321942  H -0.784987 -0.531152 -1.473704  H -1.246380 -0.652288 1.613536  H -2.402642 -1.213182 0.399606  H -0.839518 -2.045335 0.564172  H 0.501891 1.535412 0.818379  H -1.279410 1.597020 -1.172574  Freq Int   |  |  | | --- | --- | | 80.4768 190.1762 227.654 241.2618 277.0 429.784 517.8662 533.5893 567.6484 632.7064 693.9117 899.3301 995.5756 1045.4696 1133.8698 1191.8373 1231.5776 1266.9602 1291.4084 1396.9241 1434.8662 1462.5574 1471.4363 1886.6956 3015.6569 3097.8162 3124.322 3152.1864 3625.6223 3726.943 | 3.2533 2.1774 2.2878 7.4639 15.4293 4.092 16.5078 89.9563 13.2728 91.5433 69.7057 15.5347 15.1477 37.7223 81.1545 61.357 6.4773 296.7187 167.7256 13.386 0.6268 23.6522 14.0522 119.7669 33.6995 4.461 3.8344 1.066 114.663 262.3839 | |
| **1f**  O 1.236541 -1.346330 0.001668  C 0.773917 -0.238518 -0.054569  C -0.681209 0.106734 -0.374388  C -1.637860 -0.937019 0.181730  O 1.525332 0.881503 0.101841  O -1.068094 1.376480 0.121307  H -0.734005 0.090880 -1.476709  H -1.607891 -0.926373 1.273185  H -2.654079 -0.704514 -0.139691  H -1.364132 -1.931597 -0.169940  H 2.436742 0.592142 0.256922  H -0.355956 1.999061 -0.058934  Freq Int   |  |  | | --- | --- | | 45.2494 221.8376 252.5671 312.6264 344.0904 415.2072 510.0479 539.483 621.1096 732.3758 814.7579 929.4925 1047.6408 1095.8044 1157.1377 1160.9845 1288.5285 1328.4399 1368.1612 1400.8174 1425.9736 1486.9301 1501.916 1836.2841 2941.0812 3050.7327 3120.4747 3138.2462 3761.6342 3827.8001 | 2.453 2.1871 3.1854 79.961 55.9702 10.9871 9.0744 37.4709 101.0646 39.7934 8.6495 3.8703 73.2254 23.6616 176.424 117.3203 57.3022 26.5026 16.6277 41.9891 19.4609 10.8769 1.1329 248.8197 39.3992 12.8123 20.0882 11.4637 67.9706 46.1634 | | **1f+**  O 1.092106 -1.429200 0.114128  C 0.882165 -0.277634 -0.025621  C -0.776123 0.211882 -0.368290  C -1.732274 -0.857095 0.061193  O 1.628546 0.786733 -0.027441  O -0.939546 1.374127 0.287500  H -0.616832 0.323328 -1.453077  H -1.763055 -0.950397 1.148288  H -2.729421 -0.567062 -0.284247  H -1.463851 -1.815503 -0.382150  H 2.571332 0.571845 0.117012  H -0.489636 2.121581 -0.143015  Freq Int   |  |  | | --- | --- | | 53.6989 207.9717 230.6029 257.9016 351.1192 380.1238 461.4073 540.0419 550.1074 580.2172 686.0805 915.4104 1009.5326 1051.4507 1119.1225 1164.8378 1223.6555 1289.733 1310.7526 1400.6985 1439.2015 1462.4873 1474.8011 1875.6106 2979.0697 3042.4791 3113.4509 3149.117 3652.4837 3710.7076 | 0.8018 0.4809 0.5003 1.0469 13.5851 1.6329 17.867 95.6768 141.167 30.5971 68.9897 9.4755 1.8585 35.3456 35.2446 200.3849 6.2472 126.7942 43.2419 15.2304 18.5599 27.0175 9.5432 183.8612 20.3457 14.6113 2.8641 1.0325 265.4742 258.7139 | |
| **1g**  O 1.598965 -0.951765 -0.453793  C 0.811302 -0.105489 -0.125430  C -0.684856 -0.131167 -0.423942  C -1.386033 -1.042710 0.593471  O 1.152917 0.974794 0.621834  O -1.261938 1.160482 -0.478362  H -0.789559 -0.555324 -1.424096  H -1.267361 -0.647723 1.606769  H -2.451231 -1.081671 0.360467  H -0.974495 -2.054094 0.563034  H 2.101819 0.904701 0.804137  H -0.981210 1.642223 0.307655  Freq Int   |  |  | | --- | --- | | 47.4076 236.2908 239.3583 274.5577 332.0285 385.9409 523.602 589.5062 626.5779 758.5712 789.4758 910.391 1036.4575 1086.4854 1116.9334 1182.8507 1297.3447 1335.92 1352.7294 1399.6203 1427.2423 1491.6947 1497.0347 1839.2984 3031.738 3084.0097 3106.7076 3121.229 3760.7463 3816.6997 | 3.0296 0.8101 6.9767 45.6399 78.9516 8.8644 12.3416 95.146 59.4909 30.8027 16.0343 4.0378 102.2548 5.278 105.5424 177.5838 21.5886 3.0639 30.4981 13.3752 68.667 15.0979 2.9457 267.5861 12.9168 2.7514 30.4833 14.5219 67.8748 39.7244 | | **1g+**  O 1.615865 -0.881212 -0.580525  C 0.911640 -0.078320 -0.077409  C -0.792284 -0.176700 -0.459038  C -1.380457 -0.962363 0.697522  O 1.103301 0.900146 0.755156  O -1.178695 1.099024 -0.632621  H -0.771897 -0.678303 -1.424653  H -1.297440 -0.432027 1.649108  H -2.442481 -1.110148 0.467599  H -0.908408 -1.941695 0.780586  H 2.042471 0.978272 1.014960  H -1.379403 1.544532 0.209860  Freq Int   |  |  | | --- | --- | | 52.3848 201.4364 220.0858 242.8498 290.6374 428.3957 511.655 538.2472 553.8672 587.5736 688.5008 881.0466 1009.8063 1043.1949 1127.5396 1181.5133 1226.1517 1316.8346 1324.5527 1394.8389 1435.2965 1455.4031 1479.6904 1859.4832 3021.1625 3097.9608 3137.2888 3150.6062 3654.205 3693.1822 | 0.9203 2.1724 0.8906 1.0971 5.3612 6.216 7.2928 51.3856 82.7844 128.0064 68.9727 8.4883 51.3552 32.144 75.9415 101.2383 150.9636 21.5315 14.4697 7.2386 43.9326 9.952 9.7152 166.6335 22.262 8.3768 2.3327 2.8541 269.1637 215.4715 | |
| **1h**  O 1.215795 -1.135122 -0.448492  C 0.777297 -0.117227 0.030797  C -0.685226 0.069422 0.404068  C -1.333188 1.186330 -0.422962  O 1.529608 0.968289 0.282790  O -1.373316 -1.149928 0.230061  H -0.710064 0.350314 1.465412  H -1.281888 0.943491 -1.487142  H -2.384458 1.266760 -0.142497  H -0.842122 2.145580 -0.248678  H 2.434776 0.759751 0.006041  H -0.746237 -1.762951 -0.179423  Freq Int   |  |  | | --- | --- | | 45.4833 234.4355 245.9156 311.7319 328.434 405.5578 498.7558 589.8354 645.5296 746.1787 808.0324 931.0226 1050.9151 1105.408 1147.2173 1191.1334 1275.6557 1348.5135 1353.8127 1404.9757 1444.102 1494.303 1501.3946 1812.3839 3003.7211 3040.0118 3112.893 3123.9097 3738.3239 3753.9788 | 4.3853 3.3193 1.3898 37.7257 45.4126 12.2456 14.2502 58.2216 42.6424 53.4157 27.5481 0.8899 57.2936 35.1253 253.5999 45.6343 35.3338 88.4542 5.867 12.2991 12.8776 12.5971 2.9736 288.3337 25.2259 15.0914 23.4253 16.0012 83.679 66.0608 | | **1h+**  O 1.098054 1.400559 -0.166436  C 0.906772 0.249035 0.015408  C -0.765407 -0.211087 0.373875  C -1.714409 0.880626 -0.022410  O 1.656388 -0.803203 0.059788  O -0.913112 -1.428671 -0.172824  H -0.572154 -0.329893 1.449922  H -1.761173 1.010556 -1.107252  H -2.710708 0.610354 0.341906  H -1.423078 1.828998 0.428472  H 2.598406 -0.580238 -0.076923  H -1.423674 -1.400698 -1.001584  Freq Int   |  |  | | --- | --- | | 22.9075 216.0463 232.1739 258.1062 349.5498 371.3766 448.0133 540.9119 554.6236 600.3557 690.133 912.138 1012.726 1044.1692 1135.1633 1169.371 1217.9584 1314.3047 1328.1063 1402.9407 1428.7104 1467.6678 1475.4154 1870.573 3011.1568 3035.3266 3101.8588 3141.388 3653.0861 3693.8609 | 2.7365 2.1792 2.9453 1.0242 14.3485 5.204 1.2217 75.504 38.4419 202.5511 60.7537 22.0201 14.4273 38.2716 39.8814 146.4504 171.5996 21.6036 2.9786 17.231 57.6189 13.5962 7.2681 205.5936 30.7733 8.0544 2.8476 1.5547 276.0829 226.6369 | |
| **1i**  O 1.346387 -1.232027 -0.147985  C 0.804437 -0.156777 -0.076071  C -0.677782 0.041515 -0.377451  C -1.511042 -1.040605 0.312291  O 1.453394 0.975147 0.242233  O -1.069830 1.351848 -0.003697  H -0.755674 -0.089035 -1.468492  H -1.467859 -0.910077 1.396000  H -2.555638 -0.968683 -0.003589  H -1.136699 -2.032798 0.058831  H 2.377482 0.719237 0.385647  H -1.994898 1.456808 -0.245421  Freq Int   |  |  | | --- | --- | | 15.3693 234.4209 246.7924 262.3683 325.7109 417.7209 515.3397 549.6574 645.9404 748.1626 812.0235 918.5838 1047.7823 1109.3905 1150.3666 1182.3585 1249.6113 1340.1586 1364.7493 1404.3828 1440.7236 1490.6803 1503.633 1816.8008 2964.6957 3034.8907 3100.1212 3129.883 3749.1736 3836.7439 | 5.5472 1.4372 115.5861 5.0277 5.4424 3.8396 1.0098 42.8176 89.0502 53.1484 13.2807 9.561 8.0948 20.0868 97.6893 318.1649 37.3398 15.7095 29.9116 14.5323 9.8616 7.8964 9.1419 263.539 34.4743 19.0413 25.0496 10.9183 56.6994 25.9264 | | **1i+**  O 1.098904 -1.400558 0.164404  C 0.906794 -0.248854 -0.015486  C -0.765521 0.210380 -0.373983  C -1.714063 -0.881044 0.024270  O 1.655733 0.803959 -0.057819  O -0.913544 1.428765 0.170806  H -0.572711 0.327569 -1.450291  H -1.760401 -1.009386 1.109328  H -2.710579 -0.611624 -0.340065  H -1.422546 -1.829984 -0.425296  H 2.597877 0.581287 0.078505  H -1.423648 1.401919 0.999887  Freq Int   |  |  | | --- | --- | | 23.1818 216.1094 232.2807 258.2364 349.587 371.6573 447.9918 540.8614 554.75 600.4006 690.0928 912.1376 1012.7663 1044.1399 1135.1132 1169.4038 1218.0498 1314.3478 1328.168 1402.9707 1428.7006 1467.6657 1475.4324 1870.4234 3011.1259 3035.3171 3101.8348 3141.3729 3653.0732 3693.8636 | 2.7474 2.1837 2.9373 1.0227 14.3102 5.2687 1.2482 74.7617 39.0917 202.4518 60.8916 21.9977 14.4201 38.2246 39.7672 146.4155 171.7228 21.5659 2.9828 17.1926 57.5803 13.618 7.2692 205.5061 30.7707 8.0561 2.8467 1.5617 276.0333 226.7221 | |
| **1j**  O -1.228199 -1.133874 0.549166  C -0.790523 -0.170435 -0.012390  C 0.663533 0.083868 -0.389163  C 1.257653 1.192456 0.489759  O -1.559158 0.884967 -0.390391  O 1.350035 -1.143631 -0.242197  H 0.661972 0.416520 -1.436923  H 1.253703 0.877574 1.535758  H 2.291999 1.389395 0.192907  H 0.691802 2.120331 0.390878  H -2.462004 0.683303 -0.103437  H 2.277133 -0.982151 -0.441033    Freq Int   |  |  | | --- | --- | | 50.3731 230.6004 241.5489 246.5761 309.7663 395.9486 500.4384 588.0815 632.7467 748.0431 802.179 920.715 1047.57 1100.7629 1115.501 1180.0659 1250.4127 1323.2644 1351.7282 1401.7283 1436.68 1493.112 1504.4819 1857.8847 2987.755 3031.3453 3097.39 3121.5608 3762.8917 3839.3824 | 0.3512 97.7175 10.6217 12.7919 2.0212 2.8331 12.613 72.9096 63.4574 38.7665 6.0785 14.6106 6.5457 21.1585 389.2365 16.1786 22.21 11.0117 17.2175 9.1429 14.6366 7.5569 16.8414 288.3523 34.9601 18.2431 23.7643 15.5964 62.1829 30.3308 | | **1j+**  O -1.098304 1.400709 0.163919  C -0.906352 0.248866 -0.015574  C 0.765098 -0.210254 -0.373978  C 1.713986 0.880721 0.024748  O -1.655713 -0.803717 -0.057185  O 0.912956 -1.428952 0.170258  H 0.572385 -0.326800 -1.450440  H 1.759994 1.008948 1.109863  H 2.710532 0.611051 -0.339279  H 1.422924 1.829865 -0.424740  H -2.597810 -0.580586 0.078738  H 1.424068 -1.402801 0.998745  Freq Int   |  |  | | --- | --- | | 23.4401 216.4268 232.722 258.8102 349.7928 371.9355 448.0982 540.9455 554.7866 600.3149 690.2536 912.2171 1012.8972 1044.1303 1135.0844 1169.5102 1218.0375 1314.4691 1328.1165 1402.9108 1428.6601 1467.7016 1475.4715 1870.0389 3010.4364 3035.2583 3101.7586 3141.1497 3653.0548 3693.8199 | 2.7499 2.2186 2.9324 0.9945 14.4488 5.2942 1.2694 74.6101 39.2895 202.2711 60.8857 21.9375 14.3061 38.3036 39.7317 146.2553 171.8612 21.4711 2.9939 17.3863 57.3624 13.6459 7.2471 205.4561 30.861 8.0566 2.8329 1.572 276.2319 227.1327 | |
| **15a**  C 0.013406 0.062191 0.009561  H 0.020461 0.110247 1.10024  H 1.044795 0.111939 -0.34499  H -0.410592 -0.899209 -0.29208  C -0.810384 1.191097 -0.572974  H -0.819753 1.164082 -1.664757  H -1.843583 1.162426 -0.220147  O -0.195788 2.431549 -0.135984  C -0.709459 3.606649 -0.498748  O -0.244868 4.660694 -0.16849  O -1.812483 3.471921 -1.280919  H -2.10051 4.371223 -1.484224  Freq Int  72.7906 0.4366  122.7401 2.4833  213.5558 0.5525  259.381 1.2613  375.5794 6.8468  566.3121 11.2772  568.8814 100.5894  616.3792 27.8832  786.8873 43.8483  822.1073 0.101  854.5933 0.5401  994.7282 3.3974  1084.4135 102.4151  1125.9609 103.6852  1177.4185 3.9981  1188.609 375.0637  1304.8713 0.6698  1365.6467 168.9206  1410.7081 45.2975  1434.9279 7.8665  1483.8696 7.3019  1501.7859 3.4432  1523.3724 1.0888  1862.4073 606.9941  3040.0751 14.6909  3050.8591 20.0257  3090.3897 6.2652  3107.7105 25.5747  3120.7031 39.0277  3806.3625 90.867 | **15a+**  C 0.047371 0.050209 0.027063  H 0.03658 0.108986 1.115604  H 1.071268 0.116813 -0.341327  H -0.352878 -0.928202 -0.262523  C -0.838367 1.083389 -0.596484  H -0.816521 1.102578 -1.684504  H -1.858525 1.094803 -0.217327  O -0.250459 2.464482 -0.171667  C -0.763019 3.549015 -0.529443  O -0.208533 4.645959 -0.130924  O -1.818909 3.625283 -1.277191  H -2.116766 4.531492 -1.484789  Freq Int  30.6257 0.9732  99.1629 12.9655  164.409 0.6531  252.7019 1.7759  323.2535 20.7168  431.3816 11.2095  452.5812 167.4061  539.2138 55.9126  720.1544 90.0695  752.0138 19.2369  814.678 2.1822  943.3224 89.1369  1056.6722 27.5512  1114.5301 0.323  1125.8106 8.7394  1147.0662 161.5208  1277.3982 1.1794  1371.1755 105.0358  1410.1395 37.2784  1452.9881 229.9675  1456.6351 14.2957  1490.8014 2.1723  1498.9017 5.616  1654.4209 289.5051  3035.4788 23.2391  3097.9821 0.8435  3110.7084 11.4721  3141.0449 0.7792  3177.636 0.8096  3676.9844 347.8997 |
| **15b**  C 0.032392 0.098542 0.023019  H 0.039245 0.149755 1.113751  H 1.063774 0.151534 -0.331688  H -0.385672 -0.866633 -0.274488  C -0.798842 1.218672 -0.564697  H -0.812222 1.192331 -1.656657  H -1.833562 1.190517 -0.215672  O -0.199084 2.467839 -0.138068  C -0.808821 3.571027 -0.568952  O -1.790464 3.625534 -1.264925  O -0.140441 4.639116 -0.094091  H -0.611516 5.413473 -0.427228  Freq Int  52.5628 0.0251  145.5979 4.6635  202.2006 2.7464  262.878 1.0219  376.8613 14.4595  524.787 26.3716  553.1964 105.4104  670.1639 6.4156  795.8568 37.4296  818.0571 2.6045  882.6792 4.1086  1003.4835 10.5899  1095.2664 47.3456  1138.0186 9.7657  1181.8678 4.752  1210.9117 611.8233  1301.0199 1.1606  1381.1386 117.0123  1416.2616 99.9355  1443.5308 60.6335  1485.3806 7.206  1501.7425 2.5023  1525.9457 9.9057  1827.4186 404.5025  3039.39 14.467  3052.1097 16.7688  3088.5713 4.615  3107.0254 25.641  3118.1422 40.2064  3811.715 95.3264 | **15b+**  C 0.04573 0.087749 0.032522  H 0.03636 0.158908 1.120534  H 1.06883 0.160612 -0.337447  H -0.345996 -0.895528 -0.24603  C -0.843598 1.117639 -0.596043  H -0.822467 1.123527 -1.684789  H -1.863554 1.121841 -0.214577  O -0.256727 2.493998 -0.178823  C -0.742322 3.605856 -0.522165  O -1.785902 3.680831 -1.261608  O -0.160213 4.681696 -0.108964  H -0.575351 5.514575 -0.402306  Freq Int  14.1593 0.6444  109.9291 3.1331  142.3933 3.3533  252.984 0.0006  316.8162 21.0968  427.347 17.3012  429.6579 170.7509  471.8101 46.4851  740.9209 33.8991  742.5858 24.1142  814.2337 2.2404  952.7303 62.3307  1057.2462 7.5784  1123.7768 19.5376  1148.0855 10.6268  1155.208 243.3512  1291.8426 2.3062  1376.3348 101.119  1419.3084 53.5628  1448.5299 132.402  1472.9254 15.2769  1490.464 34.0314  1495.5346 10.0337  1522.2225 262.6514  3046.881 3.3162  3092.4803 0.8694  3115.9469 2.2598  3135.2482 0.5135  3169.9271 1.092  3686.4408 368.5102 |
| **15c**  C 0.040844 0.110882 0.029871  H 0.045368 0.155181 1.121107  H 1.073116 0.158642 -0.323566  H -0.381524 -0.850555 -0.272909  C -0.784299 1.237869 -0.554431  H -0.795364 1.216827 -1.646249  H -1.819314 1.213392 -0.206899  O -0.183333 2.485748 -0.123959  C -0.795497 3.610684 -0.556982  O -1.768612 3.662154 -1.249289  O -0.147718 4.69314 -0.093289  H 0.601482 4.396396 0.439126  Freq Int  45.3211 3.6483  146.7002 3.3626  199.4101 7.3847  263.7023 0.8705  372.2927 9.0112  514.9501 115.9579  523.3273 1.5909  679.5141 2.0523  783.757 25.8704  815.4231 0.0766  879.2659 23.341  997.7569 21.6695  1084.3284 95.2886  1136.486 12.8289  1181.5802 3.8362  1201.2334 160.7526  1299.6069 1.0112  1334.3485 618.3359  1405.3004 62.2526  1432.6623 25.1481  1486.3472 7.5855  1501.5669 2.6118  1526.1299 10.0097  1881.3336 369.9797  3038.6557 14.3377  3055.4657 15.2313  3090.763 1.4086  3107.1559 25.0738  3117.4612 43.2871  3799.8308 68.3676 | **15c+**  C 0.038241 0.077651 0.027956  H 0.026618 0.128509 1.117174  H 1.063336 0.131966 -0.339943  H -0.37441 -0.892069 -0.267941  C -0.82813 1.134526 -0.585948  H -0.803414 1.160561 -1.674155  H -1.848148 1.157079 -0.205767  O -0.213642 2.500906 -0.145514  C -0.684743 3.62948 -0.477975  O -1.73481 3.685748 -1.224852  O -0.172909 4.744676 -0.111145  H 0.617157 4.631325 0.450643  Freq Int  30.3189 1.3512  122.5231 9.2727  149.5309 6.4266  256.3946 0.8983  320.3213 15.1893  440.8984 19.4494  462.9644 159.7791  499.6355 2.0679  724.9341 138.0399  743.3135 29.8746  816.2431 3.0346  949.3041 69.6814  1050.2691 42.5097  1121.3332 3.6326  1146.1705 8.8442  1151.6633 105.3411  1289.6933 2.0814  1371.0307 184.1181  1418.4859 39.7982  1473.5644 15.7406  1482.2032 154.9793  1494.0189 1.9332  1506.491 111.9256  1628.438 376.6739  3046.3535 3.1396  3094.4943 0.5616  3114.5087 2.3638  3135.5141 0.9553  3172.1919 0.6738  3683.3408 303.1918 |
| **15d**  C 0.030253 0.039256 0.021751  H 0.03538 0.098751 1.111238  H 1.060112 0.098806 -0.333785  H -0.387261 -0.926268 -0.274373  C -0.797224 1.165694 -0.564911  H -0.795986 1.107995 -1.660926  H -1.831091 1.108591 -0.201342  O -0.200209 2.405103 -0.141949  C -0.709852 3.612203 -0.499899  O -0.20683 4.627499 -0.137624  O -1.81342 3.598709 -1.28635  H -2.10474 2.706633 -1.50223  Freq Int  37.9882 7.0918  86.6624 0.5013  214.8243 3.5162  252.4285 2.41  333.3518 88.1218  380.6752 1.7238  563.7395 8.5046  632.6114 3.4639  772.498 20.5577  846.4845 0.1657  853.4889 3.5461  987.6013 10.5737  1089.2576 81.8398  1118.505 142.4139  1176.7619 52.7172  1177.3452 5.8444  1304.2267 534.5612  1314.2852 0.3264  1406.0299 9.6422  1429.577 11.6964  1482.9106 7.6885  1503.308 6.0614  1526.1223 1.533  1899.3626 553.9267  2987.7411 35.7957  3030.1733 30.4834  3044.8856 12.4568  3114.046 18.8252  3125.1314 19.7996  3823.05 48.9353 | **15d+**  C 0.070841 0.027225 0.074454  H 0.094374 0.174292 1.154455  H 1.084061 0.044961 -0.327156  H -0.358271 -0.960363 -0.124594  C -0.80597 1.039076 -0.601537  H -0.813412 0.947767 -1.688763  H -1.813106 1.091994 -0.186146  O -0.170891 2.418247 -0.336094  C -0.765521 3.514558 -0.533689  O -0.20571 4.550242 0.007214  O -1.852322 3.761202 -1.177738  H -2.184941 3.033773 -1.730805  Freq Int  40.6046 1.401  74.8839 1.1378  159.8133 3.268  253.5763 1.1714  325.695 16.0907  358.1294 122.1826  456.9058 33.1134  562.6186 43.3024  717.0386 64.6304  768.1718 41.1457  827.1976 2.1506  949.3546 67.195  1056.8909 32.4956  1106.8199 183.0859  1117.8519 11.3136  1137.5819 11.4286  1291.6859 1.736  1371.5019 148.5259  1416.1228 38.7985  1465.8226 15.4125  1486.7215 13.5055  1496.6953 19.6843  1553.2503 130.2063  1611.7995 409.9319  3043.7766 8.4543  3067.0832 6.864  3114.5333 4.5851  3132.8368 1.286  3155.6495 1.6044  3725.7278 207.1692 |
| **16a**  O -1.332298 1.261361 -0.003308  C -1.116488 0.076009 -0.006366  C 0.245907 -0.572730 -0.039864  C 1.391425 0.435683 0.050477  O 2.657400 -0.194552 -0.105522  O -2.108220 -0.846524 0.014409  H -2.942678 -0.353748 0.022637  H 0.295925 -1.304472 0.774222  H 0.331571 -1.148108 -0.967229  H 1.330029 0.994678 0.992049  H 1.309762 1.160761 -0.759215  H 2.815272 -0.745163 0.667419  Freq Int  45.2737 3.5174  103.972 2.8616  179.6676 0.6522  317.0218 117.1227  376.0247 9.9739  454.8738 19.9961  529.7069 30.0226  640.5008 39.3607  670.2265 87.7637  805.8654 12.8743  895.3774 2.1406  1029.0065 109.6403  1068.2804 58.445  1070.5525 30.12  1150.5914 147.9177  1174.0911 74.923  1286.9344 31.5478  1311.014 7.039  1372.0127 39.3427  1404.4085 11.3266  1434.1185 74.468  1463.2955 12.3051  1513.6253 1.7742  1823.7767 283.7904  3013.1632 42.0338  3034.7422 10.2694  3069.1034 6.5284  3111.3452 23.0701  3752.1302 52.374  3827.7637 21.9883 | **16a+**  O -0.866060 1.249532 0.296397  C -0.944007 -0.001046 0.047452  C 0.203578 -0.933373 0.280944  C 1.495462 -0.203577 0.474434  O 2.025880 0.247394 -0.685865  O -2.045897 -0.470996 -0.396386  H -2.744073 0.204933 -0.497870  H -0.055778 -1.525896 1.167532  H 0.232726 -1.636297 -0.562884  H 2.148643 -0.439776 1.305848  H 0.044167 1.458951 0.620870  H 2.932731 0.558624 -0.563635  Freq Int  57.7313 1.0584  79.3883 2.0711  248.7354 5.2601  369.9162 9.5794  470.9708 167.227  501.1216 19.2823  525.2389 4.2655  579.9795 15.8991  680.2521 4.892  714.5204 229.0506  782.5784 12.499  868.7188 30.3231  916.2401 4.4812  1003.8034 3.4627  1183.4868 104.2571  1199.4979 126.4225  1216.1422 27.4917  1225.3864 127.6739  1301.4359 113.0261  1329.1105 9.7839  1399.9721 86.5131  1452.2317 8.6393  1556.3363 230.2232  1646.6321 326.5821  3010.5975 10.6246  3058.0562 12.9379  3188.2554 1.5311  3410.1142 392.0055  3662.9549 242.8382  3795.2339 171.3505 |
| **16b**  O 1.305726 1.297340 -0.024750  C 1.137469 0.111259 -0.006066  C -0.224006 -0.565398 -0.013228  C -1.384904 0.431495 0.015773  O -2.641391 -0.230393 0.098487  O 2.207674 -0.729479 0.018103  H 1.911471 -1.646975 0.045603  H -0.291248 -1.200067 -0.906870  H -0.304840 -1.236506 0.849519  H -1.328591 1.096953 -0.852509  H -1.307877 1.055955 0.905865  H -2.826343 -0.633248 -0.755198  Freq Int  52.8259 4.7065  104.114 8.7996  180.9916 8.0541  304.3559 123.6037  371.0143 7.8405  453.3893 91.7407  459.7514 3.1692  579.183 6.6388  658.2543 8.9185  810.25 4.912  890.1804 20.7985  1030.1667 81.0063  1060.2503 2.0254  1065.8671 88.2435  1141.6027 14.8834  1164.676 16.8248  1275.3161 220.4752  1313.5311 53.5183  1343.4224 158.2326  1396.8376 9.4526  1424.6224 58.3253  1464.624 5.9802  1511.9739 1.6739  1856.9339 240.9457  3008.0468 14.4599  3027.5164 26.8298  3051.1744 18.364  3112.0476 21.7135  3807.2658 43.3177  3829.8434 23.5338 | **16b+**  O 0.860568 1.293051 -0.242358  C 0.956204 0.040319 -0.046279  C -0.185198 -0.894151 -0.351899  C -1.490470 -0.175860 -0.483913  O -2.026262 0.163817 0.708351  O 2.095113 -0.343460 0.394849  H 2.145804 -1.301531 0.551935  H 0.072950 -1.403623 -1.289461  H -0.219870 -1.662800 0.434316  H -2.135493 -0.343088 -1.338093  H -0.048254 1.498519 -0.566347  H -2.933711 0.483409 0.613465  Freq Int  60.8324 0.528  89.9052 2.4815  251.9994 0.6213  370.6058 14.4586  471.655 170.8392  506.8984 5.115  527.6015 56.1753  587.7131 9.1862  634.2612 33.7123  684.163 7.3385  790.5559 126.5338  874.4227 8.3648  921.903 9.4833  1005.8989 3.2936  1188.3062 179.6576  1194.162 155.4093  1216.2317 49.5166  1224.7366 136.9813  1308.1237 107.2687  1328.235 12.8375  1406.546 56.9212  1453.1719 20.1571  1544.8915 291.6276  1661.8688 203.5218  2990.7919 9.1005  3051.6773 11.481  3189.1365 1.4972  3448.1478 364.9388  3724.7746 193.5987  3793.0556 183.0002 |
| **16c**  O 1.301950 -1.302733 0.000069  C 1.133607 -0.116027 0.000037  C -0.223329 0.564240 0.000155  C -1.378267 -0.424298 -0.000137  O -2.574566 0.349968 0.000027  O 2.203807 0.724413 -0.000113  H 1.907443 1.642344 -0.000124  H -0.303355 1.215564 0.878220  H -0.303308 1.216039 -0.877563  H -1.310567 -1.067853 0.884908  H -1.310522 -1.067395 -0.885515  H -3.321282 -0.255379 -0.000111  Freq Int  61.8857 6.8842  104.216 6.0257  183.9901 20.1196  282.4981 126.24  369.2556 2.2349  456.1513 103.7754  461.6236 1.6184  581.5893 4.2291  660.6699 15.9482  827.0631 1.4873  893.1604 24.7352  1038.6539 2.7784  1057.4403 125.3307  1087.4211 4.806  1143.2127 18.0763  1216.0982 0.6771  1254.4069 65.091  1288.3771 253.3833  1315.6366 0.144  1367.8115 186.9582  1460.6957 18.6858  1475.7162 3.7428  1528.2533 1.07  1856.4393 241.4665  3004.5559 32.6102  3024.6359 19.3215  3034.0167 18.5702  3064.0553 33.5142  3806.3897 44.6851  3844.1331 31.7732 | **16c+** (same as **16b+**) |
| **16d**  O 1.305745 -1.297341 -0.024759  C 1.137470 -0.111263 -0.006072  C -0.224006 0.565385 -0.013256  C -1.384908 -0.431499 0.015797  O -2.641390 0.230403 0.098489  O 2.207662 0.729494 0.018118  H 1.911444 1.646986 0.045626  H -0.304826 1.236538 0.849460  H -0.291244 1.200015 -0.906926  H -1.307879 -1.055921 0.905916  H -1.328605 -1.096995 -0.852455  H -2.826363 0.633187 -0.755225  Freq Int  52.8307 4.7072  104.1111 8.8  180.9898 8.0541  304.3366 123.6069  371.0124 7.8362  453.3944 91.7338  459.755 3.1751  579.1839 6.6393  658.2543 8.9188  810.2503 4.9121  890.1853 20.7998  1030.167 81.0266  1060.248 2.031  1065.8668 88.2158  1141.6001 14.8891  1164.6758 16.8239  1275.3184 220.5015  1313.5341 53.4826  1343.4225 158.2336  1396.8365 9.4534  1424.6234 58.3267  1464.6262 5.9791  1511.974 1.674  1856.9375 240.9479  3008.0447 14.4586  3027.5236 26.822  3051.1669 18.3704  3112.0406 21.7153  3807.2588 43.3179  3829.8496 23.5351 | **16d+** (same as **16b+**) |
| **16e**  O 1.301977 1.302733 -0.000001  C 1.133608 0.116031 0.000000  C -0.223330 -0.564222 -0.000001  C -1.378273 0.424305 0.000002  O -2.574566 -0.349972 0.000000  O 2.203789 -0.724434 0.000001  H 1.907407 -1.642360 0.000002  H -0.303320 -1.215787 -0.877893  H -0.303321 -1.215793 0.877886  H -1.310558 1.067637 -0.885206  H -1.310557 1.067632 0.885214  H -3.321286 0.255369 -0.000006  Freq Int  61.8915 6.8838  104.2103 6.0265  183.9862 20.1194  282.4961 126.2394  369.2548 2.235  456.1543 103.7747  461.6286 1.6182  581.5912 4.2299  660.6706 15.9487  827.0635 1.4874  893.1677 24.7362  1038.6587 2.7775  1057.4391 125.3263  1087.422 4.8059  1143.2109 18.0785  1216.0989 0.6771  1254.4079 65.0908  1288.3787 253.3992  1315.6373 0.144  1367.8181 186.9389  1460.6965 18.6879  1475.7204 3.743  1528.2544 1.0699  1856.4425 241.4693  3004.5586 32.6062  3024.6274 19.3264  3034.0146 18.5606  3064.0454 33.5242  3806.3825 44.6849  3844.135 31.773 | **16e+** (same as **16b+**) |
| **16f**  O -0.683276 -1.268100 0.221658  C -0.911660 -0.096765 0.020349  C 0.131359 0.985981 -0.113823  C 1.508593 0.525049 0.372768  O 2.017329 -0.553855 -0.388627  O -2.166020 0.376545 -0.123736  H -2.762909 -0.384155 -0.052222  H 0.184815 1.255540 -1.174457  H -0.211823 1.875496 0.422836  H 1.453398 0.270546 1.440458  H 2.219032 1.347211 0.265426  H 1.403461 -1.286954 -0.252157  Freq Int  56.7103 1.0441  173.435 4.663  249.69 2.6416  354.3725 1.3413  478.9865 9.9572  541.2484 17.6628  557.706 183.23  640.6157 47.3215  701.565 68.0509  815.5172 14.6858  885.2194 9.6003  971.9478 11.634  1073.7029 16.5576  1088.1831 68.8544  1157.4878 310.0834  1217.8273 3.7158  1256.1406 27.5997  1322.2002 1.7957  1398.9537 7.3165  1412.1427 93.8115  1437.4013 27.1263  1454.3786 46.3907  1510.8439 2.0619  1800.7721 274.1737  2987.7315 58.3454  3038.3176 8.049  3080.4813 12.802  3084.291 32.2829  3746.7434 65.6374  3774.4661 66.9198 | **16f+**  O -0.618019 -1.253680 -0.045563  C -0.883741 -0.011359 -0.030021  C 0.161014 1.035245 -0.230812  C 1.577240 0.577289 0.198765  O 1.853266 -0.738876 -0.049422  O -2.097053 0.371227 0.128308  H -2.722126 -0.376275 0.206211  H 0.157276 1.250467 -1.308520  H -0.146195 1.954687 0.270218  H 1.721956 0.685291 1.297175  H 2.362758 1.221255 -0.224872  H 0.393710 -1.371836 -0.134387  Freq Int  108.1978 1.3137  164.5722 13.9654  304.7018 48.5252  394.1128 0.8417  498.6219 23.7831  533.5755 9.5079  665.5894 38.9897  740.1046 148.2047  742.0143 21.9155  862.2867 7.1914  909.2977 10.0388  969.9983 11.7184  1029.425 24.0121  1072.9678 74.4099  1155.2224 2.7487  1210.6803 150.2093  1241.0415 4.3524  1307.6708 9.345  1320.2067 45.5646  1336.0357 81.3392  1406.173 13.6953  1439.8833 46.8623  1596.463 299.3792  1643.8069 430.9915  2806.5023 822.7702  2865.3718 132.8041  2989.3874 6.373  3024.0454 21.9337  3115.1434 5.86  3657.1232 230.0933 |
| **16g**  O 1.000724 -1.268721 0.354912  C 0.943428 -0.091846 0.106381  C -0.198661 0.831537 0.475831  C -1.533707 0.107882 0.491788  O -1.877382 -0.174546 -0.862632  O 1.944645 0.572813 -0.515170  H 2.642163 -0.078067 -0.685959  H 0.022488 1.235468 1.470607  H -0.229496 1.674000 -0.217306  H -2.291820 0.747655 0.963167  H -1.434142 -0.811733 1.078330  H -2.519452 -0.889124 -0.869723  Freq Int  48.1798 5.1772  110.0392 2.5873  189.1218 124.203  255.8352 0.886  373.2335 3.0927  499.7988 26.0586  535.4113 27.6175  628.3404 35.2359  693.7557 101.0696  817.0497 7.5637  898.5711 7.739  999.0779 1.1988  1054.9917 22.3764  1085.087 90.3579  1160.1878 210.4229  1206.2301 74.9242  1275.5283 15.1876  1302.7631 47.1662  1322.8939 4.6365  1414.1498 54.4444  1452.3186 15.9207  1455.9576 8.7236  1515.1389 9.4871  1829.0674 276.758  2988.4561 68.8978  3040.0853 10.166  3045.4401 25.6468  3103.8222 10.5271  3751.1444 51.5164  3852.6735 35.1677 | **16g+**  O 0.445422 -1.222642 0.080752  C 0.857727 -0.061743 -0.007882  C -0.104462 1.090885 -0.187551  C -1.462437 0.620817 0.306761  O -1.657680 -0.666669 -0.295676  O 2.124497 0.241789 0.029871  H 2.689374 -0.549608 0.103925  H 0.259438 1.980112 0.329491  H -0.120638 1.311541 -1.261473  H -2.261855 1.276597 -0.062303  H -1.516365 0.555675 1.394433  H -2.092830 -1.293897 0.308387  Freq Int  121.1854 4.0935  221.1529 1.7901  283.5012 5.8292  395.7932 2.0695  480.2589 73.0932  491.4993 13.1158  555.1686 14.7684  654.3852 50.7268  712.9497 98.9711  821.6045 8.7387  889.6073 7.1393  934.3659 8.5182  1007.0941 48.9683  1036.7408 6.3946  1154.4646 26.169  1211.3388 144.2173  1226.2529 103.7335  1269.0121 51.9105  1317.8365 28.0373  1402.383 42.0838  1427.5896 42.7798  1448.0043 34.2152  1471.1417 8.6504  1591.4726 518.9463  3014.4045 37.9094  3047.8313 8.3504  3110.8428 12.3237  3124.7347 5.1846  3686.4394 322.5247  3713.04 309.1186 |
| **16h**  O 2.209544 -0.327199 -0.151786  C 1.073327 0.015780 0.025831  C -0.055908 -0.969417 0.337731  C -1.386593 -0.671521 -0.344038  O -1.878855 0.574132 0.184786  O 0.715652 1.316311 -0.013641  H -0.245572 1.390433 0.140291  H 0.297323 -1.962312 0.058708  H -0.214405 -0.967151 1.422194  H -2.098899 -1.475752 -0.132206  H -1.254907 -0.600083 -1.430274  H -2.639233 0.859855 -0.330730  Freq Int  84.4668 2.6922  198.8063 9.8525  265.4748 0.1668  337.5662 73.7939  393.7396 51.2419  484.1924 9.4273  574.1497 5.4761  704.6569 22.3773  781.4391 85.2673  825.6792 8.0996  881.9218 24.1132  960.3708 13.3019  1048.5097 38.1028  1083.1761 9.4742  1170.7321 12.8083  1245.5863 36.2807  1254.4496 92.7356  1307.5897 12.1667  1362.3342 1.0299  1434.4604 302.6523  1444.5673 9.7154  1456.6236 10.6581  1526.5216 2.0794  1853.5881 342.1315  3008.2437 42.8266  3035.7038 8.7617  3054.7154 40.0348  3117.5227 6.2152  3575.9004 339.6246  3841.7871 49.0847 | **16h+**  O 2.143956 -0.328940 -0.166645  C 1.005952 0.105164 0.018854  C -0.021834 -1.033181 0.322419  C -1.370720 -0.701108 -0.311671  O -1.748960 0.596937 0.152137  O 0.649581 1.325314 0.005517  H -0.361402 1.366637 0.115566  H 0.361033 -1.995437 -0.015670  H -0.066553 -1.034801 1.418937  H -2.069136 -1.469257 0.047883  H -1.337133 -0.742619 -1.404942  H -2.563808 0.903738 -0.267458  Freq Int  109.5561 0.5556  216.3661 5.3807  280.3116 4.8979  333.6081 28.5444  402.5763 44.9597  486.4673 22.7571  510.1982 29.6513  649.9464 74.9556  685.095 14.9952  861.6017 86.4235  868.9954 22.5749  959.9745 89.5617  1021.8751 55.2298  1052.6665 59.8923  1146.9439 26.7442  1209.3777 21.135  1219.6423 17.7652  1273.4661 62.5505  1324.2214 3.9937  1403.0869 12.853  1433.0072 29.2477  1466.2012 82.9099  1499.3033 179.2552  1613.9066 140.6014  2852.6087 256.0613  3000.8833 199.492  3036.4925 20.2341  3068.9735 8.5866  3140.7034 11.4474  3797.8811 235.8972 |
| **16i**  O -2.222482 -0.321253 0.077176  C -1.075043 0.013669 -0.026618  C 0.057460 -0.984469 -0.289704  C 1.396667 -0.648810 0.368960  O 1.920224 0.615492 -0.081163  O -0.708838 1.309034 0.054066  H 0.261144 1.383583 -0.038033  H -0.296587 -1.961861 0.042685  H 0.191233 -1.050079 -1.377207  H 2.123197 -1.446272 0.186296  H 1.282338 -0.541466 1.448727  H 2.252946 0.507578 -0.978923  Freq Int  86.4022 4.5708  201.963 5.2852  264.6892 9.9699  362.3792 27.4332  403.0263 76.5197  498.3759 25.9268  572.9192 2.7972  697.8666 8.4125  816.5877 10.8057  839.4267 88.0223  877.4312 13.9553  959.1756 13.7485  1024.8052 75.2936  1058.8981 5.7239  1163.8037 38.6175  1218.8627 63.4935  1279.9028 17.142  1350.4672 3.9958  1381.2515 4.7423  1410.826 11.5268  1425.0855 322.3299  1461.1489 7.2495  1513.6587 3.2414  1852.6759 341.5712  3019.2977 9.6672  3039.7138 41.5709  3099.3772 10.6869  3106.0291 16.5845  3554.7251 355.2947  3818.2 37.5996 | **16i+**  O -2.150336 -0.323652 0.112967  C -1.000989 0.103828 -0.025878  C 0.007423 -1.038088 -0.311152  C 1.365338 -0.680298 0.350076  O 1.791503 0.615488 -0.056812  O -0.644659 1.324610 0.026271  H 0.361391 1.381743 -0.068895  H -0.375049 -1.991974 0.055783  H 0.059545 -1.084440 -1.405773  H 2.075624 -1.459585 0.055481  H 1.280710 -0.671674 1.436337  H 2.395075 0.581710 -0.810621  Freq Int  113.1962 1.6754  193.0504 1.2679  274.0414 5.2155  343.2804 41.0294  376.3551 22.1148  467.1263 4.3204  511.5833 10.7558  678.0174 5.8466  703.8587 19.1504  855.532 4.7825  868.4959 24.747  966.1456 96.5964  988.3364 171.0818  1057.4434 74.1783  1139.7582 45.8369  1182.2305 58.3097  1217.6002 19.5482  1308.2226 6.4485  1357.7034 8.3245  1378.8234 32.1171  1433.4849 165.6243  1443.1716 92.4356  1484.7165 2.4328  1617.2105 149.4007  2940.1132 186.4299  3041.2057 15.6995  3045.4886 45.1198  3121.1316 9.1549  3132.7135 16.9295  3796.4048 235.6828 |
| **16j**  O 0.632204 -1.299013 -0.256584  C 0.918775 -0.150743 -0.039964  C -0.095116 0.978039 0.060119  C -1.495579 0.533105 -0.376972  O -2.009875 -0.494466 0.445349  O 2.215514 0.194117 0.147231  H 2.289058 1.142890 0.305558  H -0.127305 1.309939 1.104728  H 0.244800 1.829638 -0.542383  H -1.465085 0.227751 -1.431584  H -2.182667 1.377702 -0.293808  H -1.430021 -1.255430 0.310418  Freq Int  61.2171 1.5486  173.9129 12.1289  251.8915 9.7759  356.1376 5.6171  459.8511 69.2784  503.4651 27.4837  565.5611 107.1483  579.4293 60.8381  670.6433 2.359  821.6684 15.2579  892.4952 2.8459  964.9583 16.6428  1068.471 23.674  1088.6495 76.9018  1145.168 53.3275  1219.3486 9.3846  1256.9092 66.2822  1295.1113 304.3147  1382.1475 122.9141  1404.0385 9.6236  1435.4643 23.4817  1451.9324 40.5121  1508.4333 2.5849  1835.4619 224.884  2995.0994 48.8862  3014.3233 15.3534  3056.004 19.5192  3084.2226 32.6573  3770.8481 73.9515  3806.5212 49.9646 | **16j+**  O 0.394841 -1.245183 -0.084533  C 0.868172 -0.107808 0.004210  C -0.068765 1.077418 0.191271  C -1.440642 0.652756 -0.309447  O -1.679041 -0.620375 0.300146  O 2.161328 0.035931 -0.044666  H 2.445717 0.960773 0.021503  H -0.088506 1.286806 1.267760  H 0.302574 1.967557 -0.322215  H -1.484771 0.584270 -1.397391  H -2.215615 1.342460 0.047643  H -2.129018 -1.239045 -0.301081  Freq Int  118.233 3.5366  223.0542 6.4472  284.9212 9.6222  393.7614 19.4123  475.1767 13.7272  486.7065 66.873  538.163 67.1185  591.6171 37.9925  695.2891 12.9832  820.9407 18.7091  899.3724 10.9333  934.9927 15.5257  1010.6379 52.3919  1039.2592 5.6513  1159.652 35.5142  1204.4531 134.3578  1226.1339 42.3167  1278.0475 52.7464  1319.4588 2.6991  1388.0372 208.4681  1406.3568 108.1389  1446.8283 24.7147  1476.6775 8.0653  1612.8196 400.416  3021.9946 25.5471  3040.7128 7.0368  3102.4156 4.7493  3115.1826 8.5023  3718.3583 381.8269  3755.8719 181.8237 |
| **16k**  O -1.013206 -1.342603 -0.133530  C -0.961050 -0.147003 -0.081211  C 0.181711 0.677561 -0.669307  C 1.519267 -0.022906 -0.498703  O 1.860139 0.060444 0.882745  O -1.976808 0.559422 0.477090  H -1.758969 1.498316 0.484083  H -0.035666 0.816927 -1.734471  H 0.240028 1.670967 -0.212865  H 2.279056 0.469528 -1.119863  H 1.412075 -1.062300 -0.824742  H 2.462915 -0.657453 1.092736  Freq Int  33.574 9.4615  105.5612 11.8064  174.0944 117.8147  262.9485 6.6197  379.0495 10.6515  467.183 108.4238  507.0244 1.7044  583.4526 4.3149  658.7527 4.1148  823.409 14.3576  896.2751 9.5004  997.7226 2.2892  1047.6039 2.1646  1081.0279 95.4768  1147.5279 22.0675  1205.874 17.4475  1274.0718 14.6106  1294.0681 279.7979  1311.3172 157.5428  1392.1263 62.6333  1447.9634 3.1213  1451.1652 12.1628  1514.4648 8.858  1860.1662 236.0088  2991.8213 67.819  3028.6879 10.1936  3054.1009 15.0331  3072.6839 26.6214  3817.6972 43.7617  3855.4744 40.391 | **16k+** (same as **16j+**) |
| **16l**  O -1.967056 -0.966976 -0.263957  C -1.155948 -0.147204 0.078145  C 0.267184 -0.422498 0.501453  C 1.307586 0.227237 -0.428952  O 2.632999 -0.112672 -0.050250  O -1.433732 1.183210 0.109096  H -2.350945 1.279650 -0.188251  H 0.403677 -0.030402 1.515505  H 0.412322 -1.501894 0.522035  H 1.157414 1.312473 -0.455253  H 1.182325 -0.153439 -1.444725  H 2.824592 0.319910 0.787707  Freq Int  34.5973 1.4665  102.3957 2.7133  188.8871 0.9701  316.4491 99.2126  373.8055 34.2389  432.7574 3.4647  582.8643 57.6453  627.8127 66.8469  725.4751 49.1914  806.8776 1.1784  890.3605 10.2147  1022.1676 6.3014  1036.4931 126.5356  1066.4423 89.2509  1145.5873 59.7811  1217.7962 180.4108  1292.6402 1.7035  1307.0799 9.1005  1362.4386 45.0609  1397.1364 0.8407  1424.0902 41.1474  1477.2936 8.9643  1520.5757 1.4412  1834.489 325.4355  3020.3094 38.0129  3034.4828 9.6898  3086.8001 22.9575  3128.1094 12.7677  3754.3896 57.321  3825.4134 24.6286 | **16l+**  O -2.048214 -0.922392 0.104619  C -1.170985 -0.097277 -0.011374  C 0.245274 -0.650283 -0.134919  C 1.350835 0.475078 0.173054  O 2.549546 -0.136571 -0.141953  O -1.310584 1.201375 -0.069649  H -2.247204 1.466909 -0.015032  H 0.363995 -1.488564 0.551568  H 0.373683 -1.013640 -1.157862  H 1.278112 0.793506 1.213440  H 1.190708 1.292651 -0.528256  H 2.963977 -0.555262 0.631441  Freq Int  41.3048 5.6023  111.5052 4.243  195.2909 2.0915  330.2296 1.2211  405.6422 103.0508  430.8461 57.4349  544.8759 40.8555  590.1395 48.9881  689.6824 117.2867  785.5791 96.536  818.8298 13.7128  831.4571 18.9822  1020.7822 77.5514  1108.119 60.3647  1136.8506 32.1724  1197.5826 249.862  1212.3434 37.7255  1264.679 7.6884  1322.6752 1.9415  1361.3741 14.8539  1369.9475 68.5439  1450.8561 15.2752  1503.0589 78.1446  1700.4422 394.4259  3070.9496 4.669  3079.9236 7.9441  3136.5211 3.173  3161.0142 10.1264  3688.8589 438.1202  3717.1649 504.6471 |
| **16m**  O 1.082880 1.330617 0.068878  C 0.977338 0.145694 -0.060526  C -0.190199 -0.521107 -0.785252  C -1.520624 0.163625 -0.465857  O -1.924010 -0.046958 0.880399  O 1.946984 -0.685138 0.404502  H 1.701380 -1.602566 0.242085  H 0.017300 -0.435863 -1.858945  H -0.254318 -1.591802 -0.556946  H -2.289105 -0.171918 -1.173729  H -1.393140 1.240369 -0.578754  H -2.228039 -0.955657 0.965864  Freq Int  37.6867 2.8274  112.2652 1.4424  237.9567 7.0288  319.5413 133.2968  381.6637 10.9106  457.2796 90.23  509.0764 11.3467  580.1713 3.1938  665.3979 5.1039  816.7533 16.8745  884.7128 4.9484  991.2077 4.6242  1025.084 41.5793  1082.5475 63.5842  1126.5966 45.2402  1201.7726 23.36  1254.304 11.1442  1291.0444 389.3959  1387.6084 65.5128  1393.4492 6.1989  1417.3528 30.6421  1457.6515 9.3881  1503.4728 6.8258  1864.0821 234.2302  3001.5923 53.7288  3014.2772 31.003  3052.1591 17.4111  3113.3784 11.0575  3821.3289 37.3191  3827.6362 24.5084 | **16m+**  O 0.407728 1.249310 -0.031152  C 0.870606 0.105018 0.012817  C -0.072271 -1.068351 0.240478  C -1.452829 -0.670346 -0.278785  O -1.716037 0.701107 0.032648  O 2.159050 -0.052522 -0.086025  H 2.436265 -0.981036 -0.046290  H 0.292544 -1.978566 -0.242308  H -0.073108 -1.248585 1.323372  H -2.235506 -1.296302 0.166353  H -1.514349 -0.732556 -1.363370  H -1.784799 0.855954 0.991417  Freq Int  117.3927 1.6455  187.0058 2.2076  297.568 1.1668  398.6167 7.0438  480.0793 39.2238  531.0449 58.6158  552.4188 29.0247  595.3077 34.089  702.6367 6.8439  821.0414 22.1275  886.3787 9.0886  934.8574 13.4013  1015.8171 7.3401  1029.4628 45.5483  1141.1437 43.1229  1199.9273 148.7956  1233.7647 58.7457  1292.3464 50.9598  1319.4677 4.3879  1388.5314 244.0028  1414.2179 28.2239  1456.3675 23.7904  1483.3693 5.1122  1609.8467 392.9909  3028.221 3.9577  3032.8218 16.3485  3097.0021 1.1904  3148.381 5.8115  3702.4296 227.8348  3756.1618 208.7284 |
| **16n**  O -1.210483 -1.189749 0.451098  C -0.951170 -0.137835 -0.072649  C 0.239322 0.111131 -0.974531  C 1.541884 -0.353131 -0.317445  O 1.843885 0.381296 0.861296  O -1.721093 0.965570 0.076552  H -2.454262 0.712011 0.658101  H 0.074086 -0.463130 -1.893111  H 0.288318 1.167764 -1.247731  H 2.359606 -0.296545 -1.047866  H 1.434998 -1.391786 -0.002986  H 2.018566 1.293757 0.609774  Freq Int  33.6882 1.0952  115.3301 0.677  225.5867 6.9015  336.5804 123.7876  399.2177 6.1306  472.7994 30.7424  557.2958 37.0878  640.6048 49.2858  722.8211 74.3063  815.039 8.8755  889.6637 4.6106  997.2836 0.7016  1031.7602 44.0561  1082.5483 52.2847  1136.6311 205.7927  1208.7077 134.8318  1255.9268 12.9915  1318.9639 2.2251  1386.9554 7.0982  1409.1151 50.7283  1420.4591 44.7607  1471.2833 10.6611  1508.6917 5.8529  1832.4255 278.0592  2997.917 64.5235  3039.0476 11.8375  3085.9512 5.768  3110.412 22.4516  3746.5655 52.0817  3822.305 21.8783 | **16n+**  O -2.021860 -0.586444 -0.466007  C -1.048231 -0.033352 0.001907  C 0.131765 -0.933617 0.336731  C 1.490797 -0.109547 0.505940  O 1.992222 0.390217 -0.668838  O -0.933163 1.237576 0.275780  H -1.742811 1.733723 0.053553  H -0.082813 -1.436348 1.285036  H 0.229775 -1.695912 -0.436933  H 2.145996 -0.884691 0.941178  H 1.337412 0.719178 1.191424  H 2.368855 -0.307640 -1.229212  Freq Int  39.3821 4.6165  113.0038 0.8288  241.7359 5.2751  336.6058 5.1276  367.9943 80.1298  477.444 32.197  528.8049 24.2895  569.8266 52.5159  687.0491 120.6756  748.4678 7.3899  821.8501 8.6414  890.6157 4.8642  960.9972 110.2444  1083.4231 160.6323  1137.8538 6.6144  1199.5161 225.6035  1220.9653 17.8979  1267.4971 7.659  1299.6069 86.4418  1364.5788 30.4404  1380.372 72.6282  1443.0523 19.6995  1475.3421 23.9601  1672.5464 337.9342  2929.3098 45.4434  3068.9839 8.2612  3132.5212 5.1964  3169.7265 5.6706  3686.8547 375.7365  3727.0787 404.4143 |
| **16o**  O -1.606132 -1.100952 -0.061272  C -0.967325 -0.099372 0.128635  C 0.249473 0.016120 1.019279  C 1.506211 0.438004 0.247459  O 1.784293 -0.418996 -0.850278  O -1.274169 1.086838 -0.450602  H -2.037649 0.924533 -1.024224  H 0.044167 0.755605 1.800710  H 0.391222 -0.955085 1.498339  H 2.353886 0.490894 0.943919  H 1.360072 1.429540 -0.181980  H 1.926211 -1.309126 -0.511792  Freq Int  53.9816 2.614  105.7986 1.1486  222.6736 10.4036  335.2712 124.0126  408.4297 6.9151  465.9247 12.8007  563.634 40.2923  617.1296 82.6733  715.8849 45.7274  813.8894 6.6675  888.0333 5.8361  992.4156 8.9366  1021.8117 58.0599  1085.2154 68.2102  1125.6766 159.1377  1230.7343 113.0018  1251.5199 17.0544  1345.3376 22.4456  1361.1485 11.4152  1395.1453 20.216  1428.3393 35.5837  1470.6631 11.3354  1512.2737 2.3738  1834.9589 310.4812  2992.7526 68.2904  3042.593 11.6315  3090.4615 1.4928  3111.4795 28.3265  3760.4851 59.7628  3819.2599 23.4027 | **16o+** (same as **16n+**) |
| **16p**  O -2.184080 -0.409400 -0.131044  C -1.047974 -0.062329 0.046060  C 0.128917 -0.964969 0.333800  C 1.436076 -0.580149 -0.379136  O 2.050951 0.574665 0.160040  O -0.687168 1.256499 0.010858  H -1.492376 1.761586 -0.178802  H 0.310317 -0.940821 1.414165  H -0.180806 -1.977567 0.069145  H 1.254405 -0.474930 -1.458528  H 2.151608 -1.394048 -0.247111  H 1.417118 1.296346 0.077947  Freq Int  36.6378 3.4645  177.9176 5.2451  243.6372 0.3015  357.9599 2.381  467.6925 19.9431  486.3943 112.2377  555.6177 47.3613  614.3966 82.5704  722.0601 44.4726  801.1551 13.9502  880.6849 12.9088  948.4013 13.9135  1071.9142 11.3333  1079.6461 47.7499  1160.6509 318.7988  1213.1566 11.2376  1255.3485 15.1584  1326.6606 13.2084  1363.5828 8.0594  1404.4456 8.2769  1441.3297 57.2517  1453.951 34.2117  1513.8939 0.9723  1841.4511 316.7948  2980.3362 61.3339  3040.4025 7.251  3084.7432 30.2377  3105.9157 10.6788  3751.594 72.6747  3805.2831 58.6528 | **16p+**  O -2.146856 -0.451643 0.272554  C -1.056353 -0.004366 0.005470  C 0.097607 -1.003692 -0.049341  C 1.458930 -0.333237 -0.475888  O 2.025500 0.350428 0.573156  O -0.768377 1.251502 -0.244465  H -1.560963 1.816386 -0.184761  H 0.194645 -1.456669 0.939766  H -0.156758 -1.790622 -0.762599  H 1.377882 0.243500 -1.396095  H 2.064719 -1.247263 -0.642685  H 2.197234 1.280148 0.354975  Freq Int  38.5931 2.5035  122.87 2.1324  241.1445 4.4617  261.9363 133.2633  337.5002 2.7295  474.6164 25.3124  534.3037 34.2132  576.2036 42.8967  692.2605 132.7766  792.3435 7.2273  822.5816 17.3626  888.2551 28.7304  926.1011 131.4468  1109.0435 4.2448  1145.255 98.0243  1197.8482 245.6733  1232.4381 59.7351  1258.3619 7.3246  1289.5218 35.4062  1344.8363 19.0005  1355.8132 18.8352  1434.6855 15.9027  1458.7757 35.8915  1693.0955 264.2842  2880.3477 132.4259  3079.9783 9.4587  3129.1266 15.6289  3137.024 8.3839  3687.5057 313.0469  3741.9739 513.6532 |
| **16q**  O 1.814475 -0.754752 -0.570771  C 0.993784 -0.120956 0.037641  C -0.223589 -0.693303 0.732407  C -1.506079 0.087023 0.480952  O -1.774355 0.021972 -0.916326  O 1.092673 1.222156 0.210539  H 1.893329 1.497363 -0.259836  H -0.331652 -1.724545 0.395431  H -0.016149 -0.705914 1.808311  H -1.377497 1.122772 0.815056  H -2.320020 -0.367342 1.062618  H -2.495054 0.626072 -1.115106  Freq Int  57.8446 0.0137  109.1057 1.05  228.6485 77.0209  267.3529 44.4603  387.7204 4.3075  484.3555 1.6162  554.1351 44.4075  607.7851 75.9408  696.4849 69.9316  813.1239 5.2633  896.3467 9.2695  984.7267 10.1427  1044.6628 56.8538  1088.9448 87.0627  1167.6084 114.018  1219.2501 111.8195  1265.6436 10.5152  1299.864 38.8208  1348.7534 22.7615  1381.7163 23.4001  1455.0945 4.2064  1458.8335 13.8585  1521.9413 4.499  1838.6722 315.9549  2983.9873 69.5249  3035.0253 34.339  3044.1668 10.6241  3117.8304 10.189  3761.1411 57.2431  3844.818 32.2356 | **16q+** (same as **16p+**) |
| **16r**  O -2.059073 -0.896397 -0.253089  C -1.164309 -0.147577 0.040002  C 0.259342 -0.547796 0.343580  C 1.317190 0.335149 -0.311959  O 2.580745 -0.190091 0.082431  O -1.350600 1.194293 0.152203  H -2.285854 1.356305 -0.042883  H 0.399556 -0.503447 1.429112  H 0.386994 -1.585081 0.035034  H 1.190349 1.372214 0.018026  H 1.199504 0.307583 -1.404502  H 3.267534 0.351328 -0.316889  Freq Int  41.1242 2.3896  104.6043 3.9059  195.5527 2.1354  267.2772 120.2783  367.3173 5.6108  440.6275 4.395  571.6538 49.4105  629.6428 76.2465  709.7771 70.0374  819.3406 2.5239  884.1657 15.8281  1027.2019 37.0506  1060.6825 35.9818  1074.9214 75.6505  1186.2945 159.0209  1232.4438 7.7983  1253.9872 84.9106  1307.1051 7.5351  1331.2958 3.1151  1365.244 67.6417  1463.7507 5.1696  1477.7956 7.6215  1532.2679 2.0234  1834.8671 330.1346  2980.8354 54.05  3033.7959 31.9183  3046.653 13.2737  3122.6911 10.0526  3753.7859 56.6708  3841.3204 29.8011 | **16r+**  O -2.048116 -0.922436 -0.104920  C -1.170970 -0.097278 0.011415  C 0.245288 -0.650194 0.135322  C 1.350816 0.474932 -0.173584  O 2.549534 -0.136377 0.142061  O -1.310672 1.201354 0.069876  H -2.247297 1.466832 0.015089  H 0.373706 -1.012718 1.158566  H 0.364009 -1.489018 -0.550494  H 1.190597 1.293122 0.526985  H 1.278160 0.792431 -1.214260  H 2.964054 -0.555726 -0.630929  Freq Int  41.372 5.6063  111.4875 4.2436  195.2966 2.0913  330.2283 1.2227  405.639 102.9662  430.8127 57.5102  544.8923 40.8741  590.1832 49.0395  689.6785 117.2335  785.5894 96.5535  818.8151 13.7206  831.4831 18.9996  1020.775 77.5993  1108.121 60.3317  1136.8214 32.1972  1197.5697 249.8093  1212.3535 37.7826  1264.686 7.6862  1322.6845 1.9474  1361.3771 14.8627  1369.953 68.5326  1450.8532 15.2788  1503.0612 78.1562  1700.4367 394.4859  3070.9349 4.6787  3079.8889 7.9406  3136.5294 3.1681  3161.0151 10.141  3688.8651 438.1699  3717.1614 504.6206 |
| **16s**  O 1.984259 -0.956633 -0.276817  C 1.157867 -0.152119 0.067039  C -0.266618 -0.456061 0.466237  C -1.310297 0.281456 -0.389191  O -2.632802 0.015453 0.053628  O 1.418874 1.178879 0.128854  H 2.341207 1.291690 -0.145868  H -0.398968 -1.537008 0.391397  H -0.412196 -0.160793 1.509520  H -1.181369 0.017176 -1.447585  H -1.169156 1.357883 -0.294683  H -2.827881 -0.910194 -0.122609  Freq Int  41.0124 3.3491  105.2769 5.1514  188.7995 0.5563  323.2975 102.8239  376.697 38.2759  434.5899 3.5096  580.0485 57.2849  628.7731 65.6806  719.037 47.59  808.4729 5.9919  891.3242 8.25  1016.3885 12.7907  1051.6793 55.5088  1070.8352 122.1026  1135.2873 137.6477  1225.6427 109.7492  1278.8146 14.0696  1325.919 4.2131  1359.7432 65.2532  1401.2235 2.4268  1422.5842 33.6352  1475.9482 9.5289  1519.8703 1.3008  1831.5503 320.8124  2992.286 52.0681  3051.2832 9.7075  3097.6893 0.6098  3119.2434 27.1736  3755.4181 58.8695  3826.2289 24.7074 | **16s+** (same as **16r+**) |
| **16t**  O 1.822357 -1.090813 -0.228253  C 1.171316 -0.138773 0.092845  C -0.252936 -0.209874 0.620635  C -1.286251 0.082521 -0.484514  O -2.611659 0.086884 0.019257  O 1.676452 1.118514 -0.060613  H 1.056263 1.773518 0.279954  H -0.404021 -1.218181 1.009763  H -0.409599 0.500368 1.438898  H -1.161901 -0.639311 -1.301208  H -1.124946 1.079533 -0.901190  H -2.845769 -0.815846 0.256862  Freq Int  31.1767 11.0109  99.029 10.5142  183.8782 8.1193  318.1501 104.2394  371.423 31.1148  444.8668 5.0003  478.2287 102.5032  622.6317 10.3837  722.1334 2.4826  807.5079 1.7092  888.336 23.6779  1009.6933 7.4899  1034.7081 17.3934  1066.5281 153.6458  1126.0218 27.2611  1218.5874 7.3693  1270.021 65.6787  1314.1065 298.74  1319.5708 57.4694  1397.4469 2.2418  1421.6627 41.1803  1490.8671 5.7193  1518.4046 1.9119  1861.1378 273.7221  3008.5801 31.9287  3040.424 21.0065  3073.1288 14.3011  3106.8603 25.9312  3812.7074 40.1542  3826.9073 28.9326 | **16t+**  O 1.910438 -1.011128 -0.227058  C 1.182490 -0.080029 0.047873  C -0.256261 -0.491231 0.411497  C -1.329199 0.278208 -0.464945  O -2.537904 0.015328 0.169020  O 1.588717 1.155790 0.061147  H 0.925261 1.782305 0.388838  H -0.370047 -1.563258 0.255361  H -0.392694 -0.274370 1.477792  H -1.288836 -0.060759 -1.501152  H -1.163444 1.355481 -0.404618  H -2.982422 -0.761008 -0.207651  Freq Int  69.822 16.1676  94.9879 12.2126  190.2001 7.3018  335.4523 0.5476  391.635 27.1754  402.6738 124.1582  503.5349 91.4391  580.7161 19.3905  674.5682 10.1554  771.748 2.1961  817.2851 26.5706  851.5185 145.5155  1018.7643 113.9463  1103.0769 41.5322  1125.0225 7.9929  1188.2949 81.1363  1223.746 81.5626  1273.6789 86.4656  1318.183 165.7656  1356.0446 19.7222  1379.3534 56.3518  1453.4969 18.0951  1498.3356 115.5542  1678.2835 512.4095  3044.5448 10.2502  3059.3346 1.5139  3122.262 4.1487  3144.7671 6.2417  3735.479 582.5647  3759.1346 95.8892 |

**Table S15.** Cartesian coordinates (Å), harmonic frequencies (cm−1), and infrared intensities (km mol−1) of isomers **19** and **20** calculated at the composite CBS-QB3 level of theory.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **19a**  C 0.681483 0.082383 -0.019335  C -0.650823 -0.037925 -0.001249  C -1.644621 1.072264 0.031456  O 1.332289 1.268999 -0.060474  O 1.527998 -0.982402 0.005682  O -1.125491 -1.362338 0.074889  H -2.290745 1.070759 -0.857198  H -2.296954 0.986534 0.907909  H -1.137008 2.036875 0.068598  H 2.232615 1.113032 0.248186  H 0.964368 -1.763658 0.110349  H -1.666884 -1.537947 -0.703858  Freq Int   |  |  | | --- | --- | | 164.6687 187.0643 224.1833 248.3891 312.4876 337.4646 374.2697 502.4752 545.0153 571.2006 631.4436 755.5825 965.9878 1056.7926 1092.0845 1218.5028 1232.2153 1247.4573 1346.872 1399.6755 1429.0271 1478.1794 1495.147 1826.8472 2987.8526 3034.2102 3117.247 3743.1323 3769.8378 3812.5724 | 33.765 3.2522 43.961 96.9759 48.0179 23.1645 39.3614 18.124 98.8816 1.0275 18.1613 20.5616 38.9748 7.9462 202.0577 184.0757 27.0266 41.5866 174.7293 71.1006 23.7996 9.4765 15.1481 160.5766 65.6679 36.7916 9.7678 71.6401 18.6807 90.9969 | | **19a+**  C 0.730155 0.084119 -0.000007  C -0.678314 -0.085024 -0.000041  C -1.667781 1.015570 0.000011  O 1.224113 1.287266 -0.000007  O 1.570291 -0.913776 0.000020  O -1.023973 -1.369567 0.000003  H -2.310792 0.946904 -0.885420  H -2.309493 0.947978 0.886479  H -1.178486 1.987396 -0.000907  H 2.197371 1.280996 -0.000019  H 1.116923 -1.775344 0.000010  H -1.983336 -1.507297 -0.000037  Freq Int   |  |  | | --- | --- | | 87.7016 138.599 250.4838 370.0027 380.4793 472.5104 524.2405 526.0497 560.9293 571.9142 666.8208 780.6896 1004.5063 1017.3074 1102.3273 1160.8317 1216.0695 1360.9495 1400.5995 1426.493 1463.5712 1472.9802 1571.4475 1683.1082 3016.3635 3066.6573 3155.7214 3700.6385 3715.4986 3763.966 | 0.2207 6.9651 3.4392 3.1167 1.1761 165.1561 204.1398 23.0463 4.4118 41.3146 14.2633 22.68 10.5915 5.9086 245.2796 42.1762 123.1204 374.1941 57.8318 93.7645 16.4846 39.5575 121.8658 120.1398 6.4694 0.498 1.8975 199.5554 345.0243 232.3404 | |
| **19b**  C -0.667160 0.087133 -0.014155  C 0.655572 -0.100314 0.008564  C 1.692205 0.971085 -0.051462  O -1.342628 1.286484 -0.016185  O -1.511321 -0.989116 -0.112645  O 1.193371 -1.370846 0.071172  H 2.281146 1.007560 0.871502  H 2.387421 0.767376 -0.872056  H 1.250528 1.953859 -0.225522  H -0.876948 1.905507 0.553725  H -2.297608 -0.799802 0.413499  H 0.456386 -1.994101 0.062444  Freq Int   |  |  | | --- | --- | | 157.9648 177.504 206.4083 246.2416 301.8298 339.7061 377.6748 447.0006 509.93 549.4837 584.4764 755.8899 975.1193 1062.1295 1082.809 1175.8108 1214.7377 1281.8043 1350.5557 1386.1874 1436.6417 1471.5063 1498.5477 1817.1874 3016.7022 3061.7015 3106.6161 3792.111 3795.836 3847.9116 | 2.3814 30.8925 31.4884 17.2486 102.4223 39.5174 21.056 122.6987 27.6786 8.2238 8.4561 3.2859 40.3477 8.8523 109.2661 233.9118 74.3714 169.8802 93.9297 85.1427 5.7555 6.4136 1.9906 28.6089 38.259 21.6079 23.9224 58.5395 42.8125 45.9517 | | **19b+**  C -0.711284 0.111534 -0.003068  C 0.682994 -0.142363 -0.008979  C 1.722186 0.918091 -0.004337  O -1.281654 1.288631 0.005702  O -1.509260 -0.927111 -0.006271  O 1.109239 -1.384927 0.005978  H 1.945135 1.235435 1.021875  H 2.641255 0.518481 -0.434073  H 1.427528 1.796439 -0.584503  H -0.659741 2.032242 0.023407  H -2.450692 -0.682254 0.001441  H 0.386540 -2.036653 0.026878  Freq Int   |  |  | | --- | --- | | 47.7865 132.2359 245.1603 361.2496 390.0169 432.116 507.9481 517.4435 567.2759 602.2999 639.1106 779.7679 996.9087 1024.4081 1108.0267 1168.2611 1183.6106 1364.5741 1407.2185 1437.1367 1464.6301 1476.6146 1550.3657 1668.9897 3019.6069 3085.5132 3133.0601 3696.7499 3722.0486 3758.8759 | 0.2756 5.7838 7.6761 0.0137 2.1467 245.8254 43.0166 16.7799 33.1604 143.0154 0.6211 8.3965 25.0776 4.7348 159.9695 16.4714 196.3563 438.8807 23.0565 33.4762 53.2426 52.9717 116.9264 54.789 8.7367 2.7002 3.1787 158.7332 367.0635 144.3745 | |
| **19c**  C 0.710263 -0.086957 0.012539  C -0.625939 0.055355 0.014695  C -1.665525 -1.016677 -0.035874  O 1.412098 -1.244314 0.015313  O 1.557486 0.960738 -0.018671  O -1.083770 1.387635 -0.068125  H -1.232816 -2.018080 -0.123269  H -2.302727 -1.021920 0.858849  H -2.321965 -0.873603 -0.901328  H 0.804857 -1.975766 0.160356  H 0.993074 1.740819 -0.124482  H -1.539731 1.605751 0.753583  Freq Int   |  |  | | --- | --- | | 112.2209 163.5555 251.87 279.4284 302.4454 345.5917 384.2304 511.3917 570.7031 575.8682 647.3832 762.2602 962.7571 1050.3315 1105.5138 1184.9273 1230.9596 1253.6737 1358.5924 1418.9317 1451.5432 1464.3439 1500.2042 1783.1079 2987.3498 3034.853 3071.188 3748.3939 3764.797 3856.8933 | 10.5809 4.1665 11.3911 60.4748 23.7552 43.707 42.8725 7.396 20.4317 125.0109 27.7439 13.699 22.4743 4.7994 54.0174 409.9411 10.6064 21.1163 174.6688 23.2428 10.4678 8.9084 10.499 238.832 58.4176 31.7461 36.8539 75.8365 18.5326 43.0652 | | **19c+**  C 0.753426 -0.100338 0.002496  C -0.658281 0.098626 0.009764  C -1.696666 -0.962687 0.005668  O 1.342767 -1.259628 -0.006935  O 1.586355 0.893372 0.007322  O -0.974972 1.391304 -0.013951  H -1.308095 -1.942035 0.289072  H -2.489568 -0.717100 0.719408  H -2.153034 -1.054062 -0.987810  H 0.731118 -2.008799 -0.035004  H 1.125025 1.749769 0.018066  H -1.929513 1.558243 -0.002782  Freq Int   |  |  | | --- | --- | | 50.1339 119.5164 263.1864 358.0828 393.8565 431.661 453.8404 532.2709 564.4982 597.1706 667.8879 791.2607 996.9119 1011.8306 1107.4676 1161.5337 1187.6034 1365.8334 1397.0539 1419.9441 1458.3663 1479.9274 1592.6415 1637.101 3015.7481 3075.9077 3116.5623 3712.0319 3764.4624 3789.2615 | 0.0907 0.0734 6.5617 12.6143 3.7928 1.6477 158.9689 7.9518 8.2661 214.2409 7.1955 2.3702 10.8962 8.8094 77.5916 269.6902 131.2714 248.275 133.787 89.3567 23.7426 31.8671 79.6804 186.2562 5.4682 1.2276 1.3546 197.9138 271.9995 133.748 | |
| **19d**  C -0.657607 0.096002 -0.003262  C 0.664358 -0.091922 0.000654  C 1.690039 0.989084 -0.011855  O -1.265134 1.320839 0.103934  O -1.508743 -0.994425 -0.099786  O 1.199160 -1.357368 0.018064  H 1.218286 1.969677 -0.043068  H 2.317008 0.926612 0.883311  H 2.348764 0.875803 -0.878961  H -1.808531 1.459824 -0.683112  H -2.117218 -0.966439 0.650472  H 0.458686 -1.976826 -0.019565  Freq Int   |  |  | | --- | --- | | 173.0071 192.1546 240.8935 303.3549 345.2955 362.7556 420.5048 517.7722 548.8302 553.4332 579.8808 753.7407 979.8368 1066.9955 1077.8531 1203.5916 1250.2246 1270.2906 1300.9238 1380.8796 1433.6394 1477.9766 1491.5078 1817.3631 3024.133 3067.7129 3140.8944 3744.9401 3755.6985 3779.9764 | 2.4806 3.3544 0.3113 70.0448 28.9323 13.9467 96.2761 109.3578 120.8503 14.2675 12.6878 3.3865 45.6139 20.3443 78.2898 269.8182 97.5902 138.0377 32.5643 40.7623 7.3037 7.8261 2.6997 10.3264 34.4026 22.1956 9.5184 33.2532 25.8434 42.3938 | | **19d+**  C -0.708579 0.106534 0.000012  C 0.689706 -0.122890 -0.000015  C 1.705363 0.951998 0.000226  O -1.148254 1.340890 -0.000554  O -1.481305 -0.964421 0.000636  O 1.136188 -1.357565 -0.000259  H 1.255054 1.941267 0.000691  H 2.348002 0.840853 0.879945  H 2.347673 0.841569 -0.879826  H -2.111706 1.445796 0.002117  H -2.437981 -0.811761 -0.002390  H 0.426982 -2.022809 -0.000458  Freq Int   |  |  | | --- | --- | | 48.0028 56.7234 175.3973 261.0908 374.4948 391.4842 393.8872 525.5268 568.0707 596.1559 627.3323 780.4058 1020.5408 1021.2111 1089.2157 1121.0614 1165.1912 1370.2275 1400.7887 1456.0053 1456.3433 1474.9466 1515.9953 1676.1753 3032.6443 3082.2966 3169.098 3709.0965 3759.6595 3774.2277 | 2.9469 0.3176 2.3218 0.1559 196.5718 104.3003 7.867 4.0784 23.3391 132.6495 5.6272 2.4116 20.7064 2.2359 147.2223 210.7384 251.0876 177.5618 26.7779 158.5058 18.3208 18.5554 148.4357 12.0188 12.1239 2.0634 1.3282 147.2746 63.2723 508.156 | |
| **19e**  C -0.679045 0.035002 -0.019539  C 0.650752 -0.090473 -0.007654  C 1.604244 1.062018 -0.028410  O -1.287654 1.261600 0.122014  O -1.531552 -1.028367 -0.138401  O 1.194902 -1.356088 0.108324  H 2.195084 1.093670 0.893833  H 2.311082 0.966447 -0.864202  H 1.075371 2.007404 -0.135467  H -1.975078 1.321729 -0.553701  H -2.081201 -1.068351 0.655031  H 2.013463 -1.377339 -0.397365  Freq Int   |  |  | | --- | --- | | 171.0555 186.2443 203.3017 224.5807 261.8248 364.7144 370.7134 425.4438 539.6637 559.0913 578.6189 752.2737 976.193 1056.6165 1086.1929 1223.9435 1233.6485 1268.9038 1308.6052 1338.3948 1415.6378 1482.3041 1489.8181 1829.2632 2991.6728 3041.2944 3138.1698 3756.9538 3769.2084 3819.666 | 55.092 31.0732 43.7568 152.5407 17.2876 9.3236 3.5372 71.1352 103.9025 19.1594 10.6488 2.573 62.4397 25.718 188.4963 117.7238 240.3367 56.8749 32.6162 33.3666 5.8713 7.7642 7.6462 24.624 56.1437 30.8305 7.3282 33.0391 31.6257 34.8997 | | **19e+**  C -0.727197 0.061911 0.000000  C 0.680624 -0.113194 0.000001  C 1.651995 1.008597 -0.000026  O -1.183738 1.293770 0.000057  O -1.482477 -1.005640 -0.000054  O 1.063563 -1.373681 0.000030  H 2.295262 0.945412 0.885338  H 2.295283 0.945352 -0.885371  H 1.155820 1.976034 -0.000063  H -2.148809 1.379794 -0.000191  H -2.437855 -0.843657 0.000160  H 2.028980 -1.462411 0.000020  Freq Int   |  |  | | --- | --- | | 73.6269 103.7965 226.5707 267.5746 382.3218 394.9178 432.1317 521.7637 531.8053 554.1265 649.8539 781.4855 1008.1062 1023.1714 1078.6592 1130.3424 1175.2037 1366.9451 1405.3403 1437.9248 1468.4071 1477.4303 1522.6228 1691.7591 3019.7133 3069.753 3162.6973 3755.9497 3759.6408 3773.4256 | 0.394 1.5541 0.0082 5.7806 64.0675 3.1731 233.8189 120.9906 9.2758 10.3215 8.9785 4.564 31.5914 5.7279 242.4286 257.6276 93.8659 129.8781 34.5778 216.6231 15.9386 7.3551 167.8061 33.6743 5.2821 0.299 1.2352 375.9073 64.3965 338.5215 | |
| **20a**  C 0.883519 0.072634 -0.024509  C -0.079030 1.005823 0.033597  C -1.520198 0.691175 -0.215440  O -1.839064 -0.616638 0.336997  O 0.681120 -1.251435 -0.206482  O 2.194266 0.369040 0.102678  H 0.207028 2.023963 0.253403  H -1.761480 0.676948 -1.289680  H -2.152594 1.450306 0.257214  H -2.680916 -0.902049 -0.032068  H -0.271227 -1.408908 -0.039488  H 2.662863 -0.465791 0.223193  Freq Int   |  |  | | --- | --- | | 95.3861 | 2.5641 | | 204.542 | 12.9593 | | 265.939 | 4.2996 | | 343.641 | 147.546 | | 363.128 | 43.3387 | | 412.861 | 52.6734 | | 524.211 | 19.9209 | | 649.556 | 10.8029 | | 681.882 | 25.486 | | 721.48 | 49.4741 | | 754.705 | 70.1516 | | 877.7 | 19.8399 | | 958.209 | 30.3094 | | 1037.67 | 16.5029 | | 1088.11 | 66.858 | | 1205.09 | 22.4337 | | 1217.9 | 189.458 | | 1253.09 | 30.8957 | | 1280.35 | 108.552 | | 1405.68 | 142.082 | | 1418.09 | 6.9835 | | 1475.39 | 136.016 | | 1519.36 | 1.3244 | | 1765.66 | 352.391 | | 2949.74 | 95.5193 | | 3029.57 | 51.7531 | | 3215.82 | 2.7895 | | 3518.81 | 307.03 | | 3808.84 | 91.932 | | 3828.17 | 19.6721 | | **20a+**  C 0.912386 0.007689 -0.000030  C -0.098843 1.013945 0.000038  C -1.549904 0.725110 -0.000267  O -1.768097 -0.678933 0.000686  O 0.675146 -1.257582 -0.000313  O 2.147760 0.402129 0.000166  H 0.233238 2.044994 0.000171  H -2.001479 1.205488 -0.883938  H -2.002170 1.206694 0.882376  H -2.704767 -0.906083 -0.001209  H -0.316151 -1.409137 -0.000283  H 2.771027 -0.347333 0.000122  Freq Int   |  |  | | --- | --- | | 74.1931 | 49.7643 | | 161.656 | 46.9193 | | 234.396 | 87.1698 | | 304.569 | 23.3519 | | 394.642 | 1.0142 | | 528.488 | 13.6483 | | 570.453 | 98.501 | | 664.041 | 39.0903 | | 689.023 | 3.848 | | 723.165 | 71.8832 | | 875.322 | 73.8225 | | 877.824 | 48.1965 | | 926.972 | 5.2905 | | 1012.14 | 4.7928 | | 1139.75 | 68.2794 | | 1192.23 | 136.637 | | 1215.13 | 82.7747 | | 1225.71 | 0.0143 | | 1323.09 | 54.8641 | | 1406.31 | 43.3167 | | 1427.18 | 55.1069 | | 1461.33 | 33.331 | | 1585.22 | 283.359 | | 1642.28 | 324.316 | | 2954.53 | 10.5234 | | 2976.8 | 0.0389 | | 3135.5 | 660.118 | | 3212.4 | 18.237 | | 3694.96 | 295.87 | | 3836.31 | 179.243 | |
| **20b**  C -0.877722 -0.083839 -0.025794  C 0.096175 -1.008603 0.029786  C 1.513790 -0.641149 -0.295080  O 1.908426 0.632157 0.291984  O -0.675861 1.231848 -0.263541  O -2.181224 -0.370524 0.158196  H -0.165695 -2.028819 0.270522  H 1.678731 -0.482135 -1.365788  H 2.201495 -1.428616 0.027383  H 1.851308 0.525682 1.249470  H 0.283398 1.398789 -0.149967  H -2.653419 0.468799 0.221790  Freq Int   |  |  | | --- | --- | | 134.809 | 5.2994 | | 205.547 | 3.0505 | | 249.233 | 8.7629 | | 348.935 | 125.869 | | 392.691 | 66.2563 | | 469.443 | 76.6833 | | 532.063 | 58.7522 | | 658.94 | 6.2514 | | 684.717 | 22.6421 | | 723.539 | 38.2105 | | 820.091 | 56.9325 | | 873.092 | 15.5385 | | 940.318 | 81.0921 | | 1007.9 | 32.2087 | | 1071.86 | 25.5119 | | 1194.13 | 67.9843 | | 1218.12 | 115.691 | | 1253.57 | 96.877 | | 1352.37 | 1.1935 | | 1394.47 | 112.888 | | 1397.81 | 55.3401 | | 1455.34 | 164.12 | | 1512.21 | 0.1309 | | 1751.02 | 357.751 | | 3023.2 | 65.6654 | | 3056.85 | 33.6478 | | 3213.82 | 3.5639 | | 3506.11 | 274.549 | | 3790.19 | 22.3719 | | 3806.72 | 96.172 | | **20b+** (same as **20a+**) |
| **20c**  C -0.883537 -0.072628 0.024518  C 0.079035 -1.005793 -0.033611  C 1.520182 -0.691124 0.215543  O 1.839152 0.616570 -0.337112  O -0.681173 1.251435 0.206550  O -2.194271 -0.369060 -0.102718  H -0.206997 -2.023918 -0.253508  H 2.152599 -1.450377 -0.256879  H 1.761354 -0.676675 1.289807  H 2.681015 0.901978 0.031932  H 0.271163 1.408946 0.039521  H -2.662873 0.465755 -0.223336  Freq Int   |  |  | | --- | --- | | 95.4209 | 2.5652 | | 204.543 | 12.9707 | | 265.851 | 4.2883 | | 343.676 | 147.544 | | 363.173 | 43.2899 | | 412.87 | 52.7202 | | 524.211 | 19.927 | | 649.553 | 10.8039 | | 681.867 | 25.479 | | 721.487 | 49.4546 | | 754.715 | 70.1758 | | 877.695 | 19.8384 | | 958.211 | 30.3316 | | 1037.68 | 16.5048 | | 1088.12 | 66.8392 | | 1205.1 | 22.4628 | | 1217.91 | 189.458 | | 1253.1 | 30.9205 | | 1280.35 | 108.525 | | 1405.68 | 142.044 | | 1418.09 | 6.9978 | | 1475.38 | 136.023 | | 1519.36 | 1.3222 | | 1765.64 | 352.395 | | 2949.72 | 95.5129 | | 3029.6 | 51.751 | | 3215.83 | 2.7905 | | 3518.85 | 306.87 | | 3808.83 | 91.9221 | | 3828.15 | 19.6604 | | **20c+** (same as **20a+**) |
| **20d**  C 0.887918 -0.016281 -0.027440  C -0.054976 -0.981536 0.017387  C -1.486923 -0.668587 -0.307261  O -1.938735 0.571225 0.303156  O 0.638018 1.279425 -0.253029  O 2.212053 -0.192564 0.164725  H 0.224101 -1.998337 0.263809  H -2.139493 -1.494213 -0.006865  H -1.651700 -0.494080 -1.375478  H -1.866275 0.455400 1.258510  H -0.325985 1.402982 -0.141323  H 2.392558 -1.138014 0.186415  Freq Int   |  |  | | --- | --- | | 136.233 | 6.2588 | | 203.439 | 3.5893 | | 246.688 | 2.9045 | | 384.43 | 70.6292 | | 396.098 | 8.7983 | | 468.135 | 155.712 | | 543.324 | 6.9176 | | 640.04 | 56.6364 | | 684.515 | 35.8604 | | 710.467 | 25.421 | | 814.082 | 79.1181 | | 880.256 | 20.8858 | | 948.623 | 81.459 | | 1016.96 | 20.7222 | | 1079.25 | 40.133 | | 1201.6 | 18.2535 | | 1209.77 | 186.673 | | 1247.28 | 133.496 | | 1352.72 | 0.8999 | | 1396.55 | 48.2543 | | 1417.28 | 73.0567 | | 1486.97 | 48.7247 | | 1511.75 | 0.1358 | | 1707.87 | 480.015 | | 3022.37 | 65.6303 | | 3054.71 | 32.9718 | | 3181.2 | 12.0096 | | 3542.14 | 257.415 | | 3790.5 | 22.624 | | 3842.7 | 62.8375 | | **20d+**  C 0.925096 0.036088 0.000017  C -0.067619 -0.997237 -0.000026  C -1.529031 -0.751948 0.000158  O -1.793590 0.640088 -0.000421  O 0.638549 1.284641 0.000174  O 2.201084 -0.209129 -0.000071  H 0.261279 -2.030655 -0.000108  H -1.963793 -1.249270 0.883498  H -1.964179 -1.250013 -0.882563  H -2.737224 0.837038 0.000862  H -0.354378 1.399798 0.000128  H 2.419274 -1.153113 -0.000171  Freq Int   |  |  | | --- | --- | | 60.8382 | 43.5403 | | 149.715 | 34.5074 | | 229.583 | 102.265 | | 307.604 | 5.4114 | | 395.531 | 10.5292 | | 497.183 | 88.1542 | | 542.783 | 9.127 | | 629.241 | 22.9628 | | 697.555 | 30.4424 | | 697.806 | 12.446 | | 873.539 | 118.221 | | 885.816 | 9.141 | | 919.261 | 7.8158 | | 1022.85 | 21.0047 | | 1149.22 | 76.0127 | | 1182.01 | 115.499 | | 1211.24 | 18.1304 | | 1226.51 | 0.0025 | | 1315.65 | 207.866 | | 1406.07 | 59.0462 | | 1431.78 | 24.5136 | | 1457.98 | 22.9018 | | 1586.94 | 384.082 | | 1625.64 | 204.461 | | 2949.2 | 14.6443 | | 2970.19 | 0.0404 | | 3182.03 | 593.325 | | 3192.75 | 65.1447 | | 3773.83 | 224.222 | | 3834.4 | 182.507 | |
| **20e**  C -0.893599 -0.006525 0.024240  C 0.037496 -0.980162 -0.023922  C 1.485972 -0.712537 0.243520  O 1.868556 0.549922 -0.367279  O -0.637086 1.293553 0.212457  O -2.224576 -0.185412 -0.127080  H -0.259909 -1.991697 -0.268436  H 2.095569 -1.521859 -0.172308  H 1.701628 -0.650465 1.321319  H 2.716262 0.817927 0.002130  H 0.317749 1.407754 0.034889  H -2.405668 -1.130823 -0.125410  Freq Int   |  |  | | --- | --- | | 100.78 | 4.642 | | 203.055 | 24.8704 | | 261.322 | 0.5232 | | 369.465 | 31.2931 | | 380.878 | 107.617 | | 417.588 | 13.7753 | | 534.005 | 10.8193 | | 634.304 | 74.3312 | | 680.954 | 36.4662 | | 705.465 | 14.2173 | | 756.877 | 105.547 | | 885.814 | 24.4832 | | 965.201 | 29.1435 | | 1045.92 | 13.8601 | | 1090.99 | 78.2915 | | 1207.17 | 121.276 | | 1222.01 | 55.6817 | | 1245.87 | 127.859 | | 1278.58 | 89.0948 | | 1422.42 | 5.9418 | | 1429.07 | 89.3491 | | 1499.67 | 41.3584 | | 1518.61 | 0.8026 | | 1721.35 | 475.048 | | 2951.77 | 91.3148 | | 3030.2 | 51.4953 | | 3184.9 | 10.8627 | | 3550.14 | 288.783 | | 3823.71 | 17.7762 | | 3844.4 | 59.8396 | | **20e+** (same as **20d+**) |
| **20f**  C -0.963652 -0.042680 0.040900  C 0.229036 -0.575767 0.323480  C 1.483576 0.216577 0.457909  O 2.406733 -0.203222 -0.561171  O -1.186962 1.285244 -0.066615  O -2.123937 -0.734670 -0.145761  H 0.303362 -1.652499 0.428167  H 1.928972 0.050090 1.450333  H 1.254805 1.284495 0.366415  H 3.249841 0.222410 -0.375995  H -2.071146 1.404567 -0.432697  H -1.926275 -1.676663 -0.181582  Freq Int   |  |  | | --- | --- | | 66.0198 | 3.9619 | | 136.974 | 59.5302 | | 224.642 | 67.0641 | | 261.38 | 72.3877 | | 291.492 | 111.673 | | 368.634 | 13.7845 | | 428.349 | 22.5475 | | 529.038 | 30.3051 | | 576.789 | 18.5275 | | 647.577 | 5.3001 | | 763.396 | 59.5215 | | 889.775 | 64.0673 | | 1006.35 | 103.384 | | 1023.51 | 43.4645 | | 1113.36 | 33.0548 | | 1188.42 | 176.979 | | 1206.98 | 54.5787 | | 1244.53 | 73.8269 | | 1270.38 | 34.2395 | | 1347.24 | 145.624 | | 1418.05 | 81.914 | | 1476.39 | 17.8529 | | 1516.29 | 1.0082 | | 1777.76 | 354.961 | | 2959.42 | 85.0643 | | 3029.25 | 32.827 | | 3166.39 | 15.7191 | | 3817.21 | 72.3512 | | 3818.08 | 39.7227 | | 3836.25 | 59.6379 | | **20f+**  C -1.056533 -0.050805 0.000012  C 0.279003 -0.506651 -0.000149  C 1.435100 0.403549 -0.000299  O 2.604064 -0.349780 0.000388  O -1.288705 1.226884 0.000139  O -2.108413 -0.821726 0.000027  H 0.469194 -1.575331 -0.000319  H 1.351465 1.082272 0.874407  H 1.351855 1.081186 -0.875928  H 3.373944 0.230189 -0.000123  H -2.240970 1.433422 0.000203  H -1.906478 -1.771323 -0.000057  Freq Int   |  |  | | --- | --- | | 61.3277 | 28.8052 | | 162.353 | 12.6564 | | 176.415 | 3.452 | | 302.422 | 104.777 | | 382.724 | 0.7403 | | 478.8 | 8.7283 | | 501.572 | 136.629 | | 567.333 | 172.25 | | 592.661 | 0.8204 | | 615.728 | 41.7243 | | 692.351 | 28.9548 | | 898.382 | 12.2943 | | 978.852 | 11.26 | | 1081.72 | 92.5384 | | 1122.52 | 168.352 | | 1169.39 | 150.585 | | 1196.59 | 0.9216 | | 1207.04 | 161.106 | | 1238.2 | 53.5862 | | 1316.35 | 99.759 | | 1373.97 | 168.067 | | 1450.92 | 62.0628 | | 1569.75 | 171.617 | | 1615 | 500.128 | | 2871.74 | 0.1602 | | 2878.88 | 96.3265 | | 3185.65 | 18.0067 | | 3698.55 | 365.662 | | 3745.36 | 260.932 | | 3827.23 | 198.601 | |
| **20g**  C 0.965019 -0.074656 -0.041976  C -0.229310 -0.605130 -0.342660  C -1.495934 0.171273 -0.493442  O -2.474578 -0.138129 0.503604  O 1.263387 1.244523 0.113379  O 2.064015 -0.831132 0.150654  H -0.274604 -1.681766 -0.443751  H -1.984792 -0.051258 -1.445692  H -1.299845 1.259649 -0.501308  H -2.002205 -0.214986 1.339290  H 0.485068 1.775379 -0.091827  H 2.815140 -0.238032 0.270665  Freq Int   |  |  | | --- | --- | | 75.6885 | 0.5182 | | 119.978 | 32.5561 | | 252.611 | 117.459 | | 265.458 | 47.5224 | | 339.876 | 98.8831 | | 396.936 | 42.0654 | | 433.387 | 11.8239 | | 530.615 | 28.9811 | | 573.783 | 13.8563 | | 655.771 | 2.7299 | | 783.757 | 28.5356 | | 871.17 | 26.0967 | | 987.375 | 110.824 | | 1018.61 | 113.926 | | 1117.8 | 13.0533 | | 1169.09 | 160.447 | | 1216.92 | 45.7564 | | 1229.52 | 109.087 | | 1322.23 | 12.4717 | | 1354.61 | 55.4921 | | 1412.89 | 101.926 | | 1439.59 | 148.821 | | 1516.67 | 5.1028 | | 1763.83 | 349.655 | | 2895.94 | 118.862 | | 3056.24 | 39.5756 | | 3195.24 | 3.1212 | | 3806.81 | 31.1001 | | 3814.02 | 17.4288 | | 3817.61 | 127.423 | | **20g+**  C 1.064225 -0.053923 -0.003262  C -0.277382 -0.498742 0.077464  C -1.458438 0.382763 0.184023  O -2.581932 -0.335667 -0.218916  O 1.465925 1.185737 -0.078556  O 1.996867 -0.951797 0.004798  H -0.431240 -1.572292 0.089769  H -1.321205 1.310441 -0.406896  H -1.519927 0.711524 1.243818  H -3.385984 0.111743 0.068715  H 0.751013 1.838606 -0.137868  H 2.890034 -0.566797 -0.065497  Freq Int   |  |  | | --- | --- | | 54.7237 | 20.2499 | | 139.813 | 2.5495 | | 187.06 | 1.5421 | | 295.181 | 126.97 | | 380.093 | 9.5299 | | 482.448 | 13.849 | | 499.959 | 186.59 | | 567.163 | 58.8588 | | 598.566 | 18.8799 | | 634.975 | 18.454 | | 705.182 | 43.4281 | | 888.01 | 30.3164 | | 976.669 | 19.8689 | | 1092.97 | 95.7781 | | 1111.74 | 179.541 | | 1159.35 | 162.464 | | 1196.24 | 129.55 | | 1208.76 | 56.3796 | | 1269.19 | 45.9385 | | 1323.36 | 26.504 | | 1404.75 | 54.8371 | | 1458.7 | 17.0113 | | 1546.57 | 249.461 | | 1620.17 | 327.942 | | 2863.91 | 42.5992 | | 2887.79 | 37.9453 | | 3199.8 | 26.6609 | | 3689.33 | 373.598 | | 3747.21 | 115.173 | | 3824.06 | 176.04 | |
| **20h**  C 0.939771 -0.043400 -0.037305  C -0.209784 -0.674340 -0.310497  C -1.507505 0.034654 -0.548573  O -2.365239 0.103743 0.602348  O 1.062725 1.297602 -0.004683  O 2.138289 -0.637533 0.221738  H -0.201134 -1.760137 -0.320382  H -2.040782 -0.443928 -1.381943  H -1.322167 1.072023 -0.826886  H -2.466137 -0.792817 0.936481  H 1.979781 1.507204 0.207004  H 2.029351 -1.594328 0.208749  Freq Int   |  |  | | --- | --- | | 50.4388 | 4.9511 | | 112.394 | 57.2789 | | 208.629 | 41.245 | | 229.88 | 147.999 | | 279.391 | 83.0025 | | 370.26 | 11.65 | | 436.897 | 11.6047 | | 544.306 | 18.7456 | | 582.564 | 14.7742 | | 655.191 | 6.0159 | | 749.286 | 82.7081 | | 873.047 | 49.321 | | 992.271 | 159.923 | | 1018.63 | 43.8611 | | 1090.65 | 26.1881 | | 1186.5 | 93.5783 | | 1198.49 | 103.484 | | 1227.51 | 80.836 | | 1347.96 | 154.016 | | 1360.1 | 5.3239 | | 1413.83 | 82.8927 | | 1459.06 | 58.983 | | 1504.13 | 0.6896 | | 1761.5 | 375.942 | | 2978.76 | 86.4858 | | 3105.29 | 10.219 | | 3147.77 | 21.6023 | | 3822.1 | 120.274 | | 3824.32 | 9.6413 | | 3837.84 | 61.9115 | | **20h+**  C 0.929719 -0.029613 -0.055433  C -0.262434 -0.716289 -0.389798  C -1.549556 0.008006 -0.605188  O -2.005478 0.128874 0.752455  O 0.938984 1.264882 -0.071140  O 2.060917 -0.603903 0.247540  H -0.261424 -1.797755 -0.308045  H -2.238870 -0.549321 -1.238885  H -1.414967 1.012958 -0.997634  H -2.575343 -0.619574 0.978418  H 1.806354 1.635600 0.173034  H 2.022502 -1.573350 0.264790    Freq Int   |  |  | | --- | --- | | 69.7109 | 2.0256 | | 110.207 | 4.4501 | | 255.688 | 6.7885 | | 358.398 | 56.3068 | | 375.071 | 96.7854 | | 506.51 | 112.505 | | 519.926 | 91.2871 | | 579.103 | 102.178 | | 593.175 | 34.5287 | | 665.426 | 8.0539 | | 776.822 | 48.6876 | | 873.931 | 25.3479 | | 972.715 | 32.6333 | | 1037.85 | 23.5075 | | 1106.2 | 35.5254 | | 1165.92 | 111.096 | | 1182.31 | 98.8964 | | 1210.24 | 115.821 | | 1347.95 | 17.7132 | | 1359.64 | 59.0608 | | 1390.86 | 76.331 | | 1503.85 | 18.4595 | | 1571.06 | 247.105 | | 1600.53 | 383.356 | | 3094.74 | 7.6156 | | 3161.45 | 0.773 | | 3190.14 | 6.2729 | | 3699.62 | 349.702 | | 3750.93 | 235.799 | | 3776.9 | 191.342 | |
| **20i**  C -0.946906 -0.073842 -0.027046  C 0.234864 -0.646779 -0.253802  C 1.500271 0.103725 -0.532333  O 2.484746 -0.076145 0.494063  O -1.115374 1.279272 0.101289  O -2.099998 -0.797236 0.090885  H 0.276122 -1.727963 -0.205789  H 1.280480 1.165834 -0.686819  H 1.975634 -0.277628 -1.439939  H 2.071746 0.186548 1.323072  H -1.878153 1.543856 -0.428776  H -2.610188 -0.436405 0.827434  Freq Int   |  |  | | --- | --- | | 69.1274 | 0.3004 | | 157.48 | 1.7572 | | 242.691 | 17.7983 | | 279.079 | 137.942 | | 350.81 | 136.051 | | 417.64 | 2.596 | | 493.514 | 109.478 | | 544.252 | 66.8222 | | 566.354 | 23.8459 | | 605.393 | 18.4343 | | 829.193 | 12.7425 | | 877.135 | 40.3871 | | 982.328 | 158.741 | | 1025.19 | 74.8415 | | 1114.66 | 5.6158 | | 1177.34 | 87.5388 | | 1216.82 | 37.1253 | | 1242.77 | 24.2181 | | 1286.13 | 187.226 | | 1346.74 | 73.719 | | 1388.77 | 27.36 | | 1429.79 | 66.583 | | 1507.71 | 0.3304 | | 1777.31 | 185.298 | | 3021.08 | 47.0593 | | 3067.64 | 33.0624 | | 3190.57 | 5.1852 | | 3771.81 | 38.7052 | | 3777.5 | 51.6556 | | 3818.3 | 14.5783 | | **20i+**  C -1.054665 -0.059835 -0.000011  C 0.281200 -0.506669 0.000001  C 1.436731 0.402693 0.000068  O 2.606280 -0.350053 -0.000042  O -1.284427 1.227783 -0.000033  O -1.994587 -0.964356 0.000004  H 0.444935 -1.578522 0.000054  H 1.353426 1.080379 0.875558  H 1.353405 1.080723 -0.875131  H 3.375093 0.231008 -0.000231  H -2.216267 1.498762 0.000014  H -2.908310 -0.636470 -0.000049  Freq Int   |  |  | | --- | --- | | 58.9862 | 14.9689 | | 168.515 | 17.4399 | | 177.374 | 1.4424 | | 296.503 | 127.934 | | 352.962 | 3.8074 | | 383.8 | 0.1082 | | 483.089 | 3.3684 | | 506.86 | 284.278 | | 575.776 | 7.9111 | | 620.064 | 33.6512 | | 675.763 | 20.2177 | | 913.968 | 9.3162 | | 969.189 | 44.7553 | | 1067.65 | 254.825 | | 1119.36 | 214.192 | | 1134.89 | 152.457 | | 1179.06 | 107.987 | | 1200.16 | 0.8895 | | 1241.66 | 32.9069 | | 1313.89 | 102.755 | | 1378.17 | 86.7778 | | 1456.1 | 30.7248 | | 1530.26 | 264.649 | | 1629.49 | 301.555 | | 2872.51 | 0.5448 | | 2879.6 | 89.9212 | | 3203.89 | 27.2193 | | 3735.72 | 66.749 | | 3749.31 | 556.527 | | 3829.28 | 184.082 | |
| **20j**  C 0.956890 -0.071175 -0.047049  C -0.253131 -0.542615 -0.345323  C -1.493387 0.291888 -0.427108  O -2.535916 -0.204930 0.421421  O 1.235959 1.265259 0.048919  O 2.027718 -0.888445 0.188642  H -0.344253 -1.608650 -0.513724  H -1.917451 0.256920 -1.434403  H -1.258314 1.338472 -0.201991  H -2.168184 -0.266861 1.308927  H 1.822831 1.396015 0.804888  H 2.781050 -0.559546 -0.318677  Freq Int   |  |  | | --- | --- | | 84.1013 | 0.6025 | | 159.389 | 1.9384 | | 236.409 | 11.7888 | | 283.728 | 154.526 | | 360.081 | 100.853 | | 423.308 | 18.1543 | | 500.582 | 82.3924 | | 515.359 | 88.7868 | | 573.327 | 45.6566 | | 606.127 | 8.2397 | | 823.482 | 23.5012 | | 894.315 | 33.0851 | | 984.417 | 149.533 | | 1024.33 | 80.7936 | | 1116.64 | 7.6233 | | 1172.69 | 82.1637 | | 1215.12 | 22.0635 | | 1243.01 | 32.6136 | | 1291.25 | 174.618 | | 1334.05 | 105.267 | | 1386.02 | 27.267 | | 1429.39 | 60.9951 | | 1510.2 | 0.573 | | 1780.65 | 180.442 | | 3018.09 | 41.7357 | | 3063.24 | 32.9431 | | 3190.45 | 4.6731 | | 3769.95 | 38.6513 | | 3776.72 | 49.5714 | | 3818.26 | 14.7325 | | **20j+** (same as **20i+**) |
| **20k**  C 0.963732 -0.071301 -0.041114  C -0.240912 -0.559931 -0.323979  C -1.480712 0.263278 -0.422509  O -2.436083 -0.242138 0.521987  O 1.231718 1.270262 0.033968  O 2.045063 -0.873960 0.192652  H -0.327626 -1.629486 -0.466156  H -1.889678 0.192322 -1.441781  H -1.244174 1.315143 -0.226276  H -3.277995 0.184194 0.335234  H 1.761776 1.425849 0.826529  H 2.799460 -0.513603 -0.290787  Freq Int   |  |  | | --- | --- | | 68.7843 | 1.9499 | | 164.046 | 6.4639 | | 234.972 | 74.5905 | | 263.149 | 28.1597 | | 287.972 | 167.04 | | 420.96 | 18.5178 | | 494.921 | 52.8516 | | 515.1 | 120.953 | | 573.641 | 51.8843 | | 605.072 | 6.7475 | | 823.582 | 27.2365 | | 892.377 | 48.957 | | 1001.72 | 48.3242 | | 1023.6 | 84.6678 | | 1113.5 | 26.6263 | | 1188.19 | 94.3588 | | 1236.76 | 100.121 | | 1245.58 | 19.6409 | | 1266.45 | 40.6322 | | 1302.11 | 199.21 | | 1357.84 | 52.4889 | | 1463.13 | 16.0737 | | 1517.46 | 1.0801 | | 1791.88 | 189.122 | | 2960.76 | 74.9998 | | 3030.02 | 35.4582 | | 3196.77 | 4.7589 | | 3769.95 | 38.8339 | | 3776.08 | 45.7255 | | 3825.86 | 10.9461 | | **20k+** (same as **20i+**) |
| **20l**  C 0.956241 -0.067471 0.022647  C -0.228512 -0.628881 0.250621  C -1.486369 0.131589 0.503440  O -2.402499 -0.127759 -0.570954  O 1.137381 1.279976 -0.130569  O 2.107542 -0.801917 -0.062629  H -0.278200 -1.709882 0.227699  H -1.262898 1.201226 0.581994  H -1.926498 -0.199139 1.456537  H -3.245966 0.267619 -0.330081  H 1.930103 1.533526 0.358982  H 2.595916 -0.507167 -0.842168  Freq Int   |  |  | | --- | --- | | 66.0344 | 1.0528 | | 159.94 | 16.5067 | | 234.767 | 76.2336 | | 262.367 | 117.448 | | 281.416 | 64.5594 | | 416.206 | 5.8372 | | 488.224 | 101.943 | | 540.918 | 93.0936 | | 567.081 | 36.6815 | | 606.893 | 18.2656 | | 828.845 | 19.655 | | 879.571 | 54.0424 | | 1000.39 | 70.2548 | | 1025.49 | 71.4398 | | 1116.03 | 21.4323 | | 1183.87 | 101.668 | | 1235.32 | 92.3566 | | 1254.01 | 19.5232 | | 1267.71 | 51.7075 | | 1300.7 | 187.454 | | 1363.46 | 54.1768 | | 1464.75 | 15.9067 | | 1515.46 | 0.8485 | | 1790.2 | 196.037 | | 2958.74 | 81.1241 | | 3032.91 | 35.8399 | | 3196.56 | 5.2323 | | 3771.74 | 39.6278 | | 3780.87 | 49.6351 | | 3823.1 | 9.9693 | | **20l+** (same as **20i+**) |
| **20m**  C 0.953237 -0.045891 0.038187  C -0.234328 -0.601951 0.308655  C -1.498886 0.174600 0.501885  O -2.493709 -0.124900 -0.488107  O 1.153735 1.286566 -0.054998  O 2.122005 -0.714775 -0.171595  H -0.295455 -1.684145 0.357044  H -1.276637 1.247579 0.524740  H -1.973050 -0.085182 1.452032  H -2.079306 0.017573 -1.345380  H 2.084179 1.430754 -0.262881  H 1.963885 -1.662263 -0.100319  Freq Int   |  |  | | --- | --- | | 62.0036 | 25.7869 | | 123.585 | 47.982 | | 212.87 | 85.6518 | | 254.023 | 55.2099 | | 353.887 | 93.8875 | | 373.035 | 18.8469 | | 429.572 | 27.1174 | | 535.964 | 4.6505 | | 574.672 | 11.042 | | 650.167 | 1.6486 | | 763.058 | 73.7536 | | 880.293 | 36.47 | | 989.327 | 191.635 | | 1022.47 | 53.806 | | 1115.22 | 22.5183 | | 1183.61 | 149.98 | | 1201.21 | 52.8402 | | 1216.63 | 37.9498 | | 1326.17 | 97.8827 | | 1375.34 | 71.1344 | | 1412.61 | 113.25 | | 1455.96 | 43.3594 | | 1509.38 | 0.3221 | | 1766.45 | 342.5 | | 3018.87 | 42.3421 | | 3064.71 | 36.8311 | | 3160.27 | 15.8582 | | 3816.49 | 12.7181 | | 3821.49 | 114.092 | | 3835.92 | 63.1195 | | **20m+**  C 0.927947 -0.031282 0.047059  C -0.253282 -0.764662 0.294960  C -1.561174 -0.111387 0.603397  O -2.080546 0.057976 -0.724615  O 0.908173 1.264000 0.153270  O 2.081768 -0.554805 -0.260292  H -0.236576 -1.829963 0.094032  H -1.463882 0.829326 1.144567  H -2.227942 -0.782008 1.139971  H -1.879816 0.948400 -1.044892  H 1.781766 1.663038 -0.011260  H 2.070334 -1.522176 -0.341821  Freq Int   |  |  | | --- | --- | | 44.6112 | 7.0402 | | 114.547 | 6.891 | | 246.219 | 13.4073 | | 333.28 | 8.7434 | | 374.064 | 127.803 | | 507.955 | 77.4998 | | 526.544 | 136.86 | | 578.3 | 97.4836 | | 592.078 | 28.0344 | | 665.162 | 7.7145 | | 780.663 | 42.7841 | | 878.874 | 17.3758 | | 965.746 | 46.7713 | | 1034.31 | 32.5874 | | 1109.33 | 35.9527 | | 1168.06 | 92.7941 | | 1185.41 | 57.4801 | | 1209.71 | 172.178 | | 1350.01 | 41.0106 | | 1364.04 | 28.7078 | | 1384.98 | 73.3841 | | 1501.61 | 25.1227 | | 1565.64 | 184.95 | | 1600.97 | 459.597 | | 3095.04 | 6.1304 | | 3161.23 | 0.9045 | | 3195.5 | 9.9872 | | 3698.39 | 331.3 | | 3744.55 | 266.597 | | 3777.97 | 142.988 | |
| **20n**  C 0.984382 -0.030035 -0.033025  C -0.202150 -0.591084 -0.335640  C -1.488627 0.150505 -0.502464  O -2.460243 -0.158940 0.501569  O 1.245692 1.284113 0.113871  O 2.135913 -0.702178 0.169971  H -0.246066 -1.671348 -0.426364  H -1.972887 -0.106613 -1.448090  H -1.316696 1.241522 -0.538346  H -1.996090 -0.159199 1.345406  H 0.443705 1.780279 -0.083595  H 1.955504 -1.644918 0.094474  Freq Int   |  |  | | --- | --- | | 74.9743 | 5.5805 | | 130.527 | 0.8217 | | 265.12 | 29.4003 | | 296.447 | 17.729 | | 358.816 | 63.2247 | | 434.746 | 14.0598 | | 451.47 | 210.79 | | 540.374 | 0.5888 | | 585.95 | 10.4509 | | 666.376 | 0.6294 | | 746.484 | 56.8668 | | 875.98 | 28.8502 | | 998.22 | 122.208 | | 1020.59 | 72.486 | | 1120.34 | 7.8177 | | 1170.46 | 327.024 | | 1210.61 | 32.683 | | 1233.75 | 14.2361 | | 1329.82 | 8.3294 | | 1362.9 | 105.321 | | 1423.54 | 63.6462 | | 1468.34 | 40.1503 | | 1517.54 | 1.1607 | | 1721.91 | 451.979 | | 2907.75 | 107.428 | | 3059.21 | 38.1688 | | 3158.65 | 12.7533 | | 3812.7 | 13.6504 | | 3821.4 | 45.3837 | | 3843.51 | 71.1496 | | **20n+**  C 1.083033 -0.034397 -0.007265  C -0.262475 -0.487276 0.056024  C -1.448698 0.390123 0.155559  O -2.573993 -0.359434 -0.178572  O 1.451739 1.208889 -0.065350  O 2.101715 -0.835778 -0.004172  H -0.445825 -1.557628 0.058841  H -1.332449 1.283428 -0.490898  H -1.486568 0.777283 1.196557  H -3.377511 0.114351 0.065428  H 0.715678 1.835844 -0.125541  H 1.859828 -1.773387 0.054459  Freq Int   |  |  | | --- | --- | | 51.8759 | 33.7928 | | 126.491 | 4.075 | | 185.319 | 8.2957 | | 297.524 | 115.953 | | 379.777 | 8.1065 | | 457.668 | 1.5287 | | 483.84 | 8.3042 | | 544.849 | 69.3126 | | 607.641 | 198.968 | | 638.576 | 20.3738 | | 689.339 | 1.9533 | | 887.732 | 14.3821 | | 979.962 | 13.1063 | | 1098.45 | 37.8398 | | 1114.26 | 141.555 | | 1161.37 | 329.628 | | 1184.89 | 29.9274 | | 1205.53 | 45.2164 | | 1262.29 | 66.4238 | | 1328.71 | 16.0744 | | 1400.46 | 119.338 | | 1457.95 | 42.9653 | | 1560.05 | 411.922 | | 1596.43 | 185.886 | | 2862.93 | 43.6861 | | 2885.06 | 34.9423 | | 3178.93 | 16.726 | | 3758.34 | 323.182 | | 3768.28 | 58.1012 | | 3823.26 | 181.116 | |
| **20o**  C 0.944447 -0.070682 0.024714  C -0.223445 -0.665791 0.262405  C -1.500992 0.064546 0.544072  O -2.408412 0.085515 -0.567154  O 1.085804 1.282556 -0.094139  O 2.110383 -0.774103 -0.102360  H -0.232086 -1.749332 0.224544  H -1.293118 1.110493 0.766832  H -1.993857 -0.378152 1.421665  H -2.575608 -0.827858 -0.819471  H 1.878190 1.548215 0.389886  H 2.594211 -0.423552 -0.861384  Freq Int   |  |  | | --- | --- | | 61.1978 | 5.3055 | | 153.789 | 2.0464 | | 224.157 | 60.1751 | | 268.333 | 106.401 | | 305.007 | 140.823 | | 417.743 | 3.6602 | | 493.62 | 105.99 | | 547.112 | 92.9322 | | 577.75 | 12.399 | | 608.225 | 15.029 | | 824.744 | 25.0516 | | 873.211 | 45.0728 | | 1001.98 | 163.031 | | 1006.49 | 40.7601 | | 1090.49 | 6.6426 | | 1171.41 | 54.5924 | | 1225.86 | 98.2171 | | 1243.91 | 26.5495 | | 1295.45 | 221.242 | | 1360.07 | 22.779 | | 1380.04 | 38.0176 | | 1431.98 | 56.7103 | | 1503.98 | 0.3828 | | 1780.22 | 203.206 | | 2973.81 | 84.2379 | | 3111.58 | 12.7123 | | 3174.43 | 8.3447 | | 3771.56 | 38.6471 | | 3778.95 | 52.8691 | | 3823.79 | 18.2348 | | **20o+**  C 0.923343 -0.041305 0.061378  C -0.266655 -0.729537 0.387845  C -1.558291 -0.016294 0.601740  O -1.981937 0.163584 -0.760844  O 0.926467 1.261140 0.104313  O 1.968852 -0.758375 -0.245432  H -0.232485 -1.808202 0.292569  H -1.440939 0.972188 1.039077  H -2.262052 -0.601963 1.192421  H -2.504952 -0.598836 -1.045388  H 1.750607 1.699305 -0.161057  H 2.792388 -0.270476 -0.407697  Freq Int   |  |  | | --- | --- | | 75.5296 | 6.4966 | | 114.669 | 4.8206 | | 254.589 | 21.3302 | | 347.436 | 18.7089 | | 372.389 | 18.1823 | | 387.612 | 103.083 | | 514.527 | 204.909 | | 526.006 | 158.577 | | 594.174 | 11.5432 | | 635.808 | 7.9656 | | 801.52 | 35.733 | | 872.616 | 6.0743 | | 972.597 | 35.8647 | | 1034.61 | 40.0532 | | 1097.75 | 55.3362 | | 1129.93 | 175.637 | | 1172.24 | 214.096 | | 1197.47 | 28.0886 | | 1346.63 | 9.2922 | | 1361.38 | 46.2727 | | 1390.64 | 28.3142 | | 1505.31 | 41.4269 | | 1544.48 | 240.749 | | 1608.45 | 260.677 | | 3095.13 | 8.8178 | | 3160.9 | 0.9675 | | 3208.29 | 12.0981 | | 3734.31 | 89.0477 | | 3749.85 | 512.507 | | 3778.27 | 145.954 | |

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